

Algorithmic Issues and Applications of BOUT to Simulation of Realistic Tokamak Configurations

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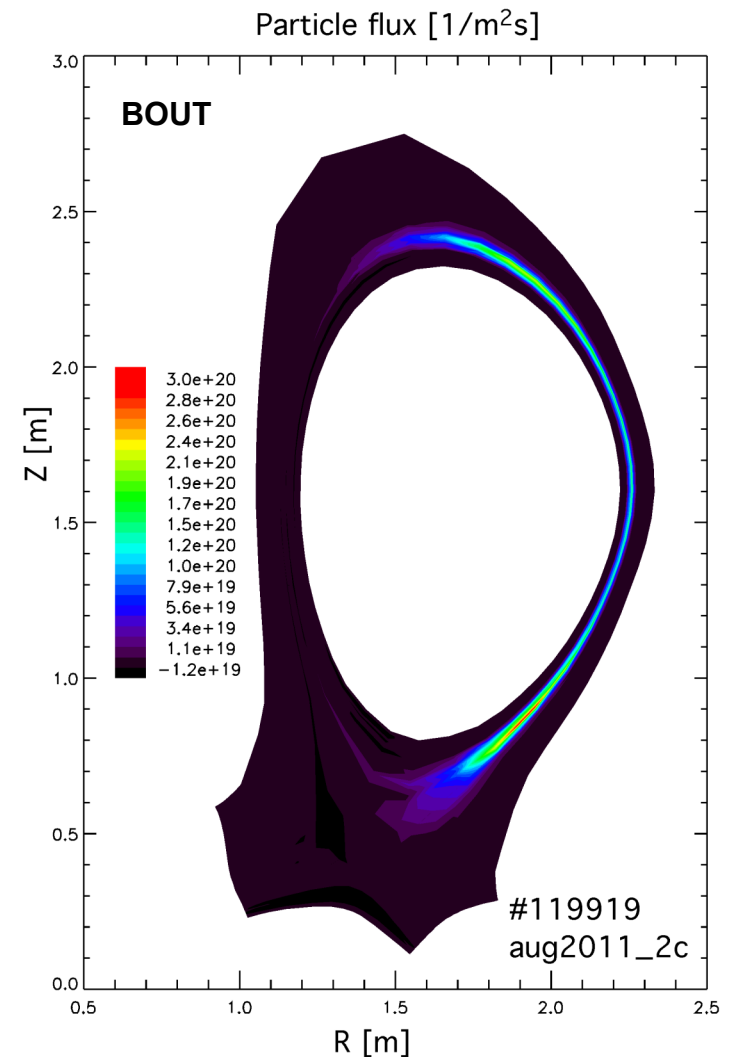
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La Jolla, CA



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BOUT Simulations of Resistive Ballooning Turbulence in Edge Region for DIII-D Shot #119919

- Simulations of electrostatic resistive ballooning in DIII-D shot #119919, with full geometry and magnetic shear, crossing the separatrix
- Nonlinear BOUT equations for ion density, vorticity, electron and ion velocities, Ohm's law, and Maxwell's equations.
- In earlier work, we have suppressed a spatial odd-even mode ballooning along the field line by either filtering with ∇_{\parallel}^2 or $-\nabla_{\parallel}^4$ diffusive operator added to right side of vorticity and ion density eqns, or with use of a staggered mesh for ∇_{\parallel} representation. Parallel damping included here; no odd-even mode seen.
- **Simulation results with/without T_e fluctuations**
- **BOUT obtains steady-state turbulence with fluctuation amplitudes and transport that compare reasonably to the DIII-D data.**



BOUT Simulation of Resistive Ballooning Turbulence for DIII-D Shot #119919 - Outline

- BOUT algorithmic issues -- control of an odd-even numerical contamination
- Electromagnetic simulations of resistive ballooning turbulence in single-null DIII-D geometry:
 - Case #1: No T_e fluctuations
 - Case #2: With T_e fluctuations
 - Case #3: With T_e fluctuations and electron parallel thermal conduction
 - Case #4: With T_e fluctuations, electron parallel thermal conduction, and $\nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$ in the vorticity eqn.
- Comparison to probe data for DIII-D shot #119919. Shot #119919 is a well-characterized L-mode shot exhibiting steady-state turbulence.

BOUT06 produces expected ballooning-like turbulence in full DIII-D X-point geometry

- BOUT solves Braginskii-like fluid equations for fluid turbulence in various geometries

$$\frac{\partial N_i}{\partial t} + (V_E + V_{\parallel}) \cdot \nabla N_i = \left(\frac{2c}{eB} \right) b_0 \times \kappa \cdot (\nabla P_e - N_i e \nabla \phi) + \nabla_{\parallel} (j_{\parallel} / e) - N_i \nabla_{\parallel} V_{\parallel i}$$

$$\frac{\partial \varpi}{\partial t} + V_E \cdot \nabla \varpi = 2\omega_{ci} b_0 \times \kappa \cdot \nabla P + N_i Z_i e \frac{4\pi V_A^2}{c^2} \nabla_{\parallel} j_{\parallel} \quad \text{vorticity}$$

$$\frac{\partial V_{\parallel e}}{\partial t} = -\frac{e}{m_e} E_{\parallel} - \frac{1}{Nm_e} (T_e \nabla_{\parallel} N_i) + 0.51 v_{ei} j_{\parallel}$$

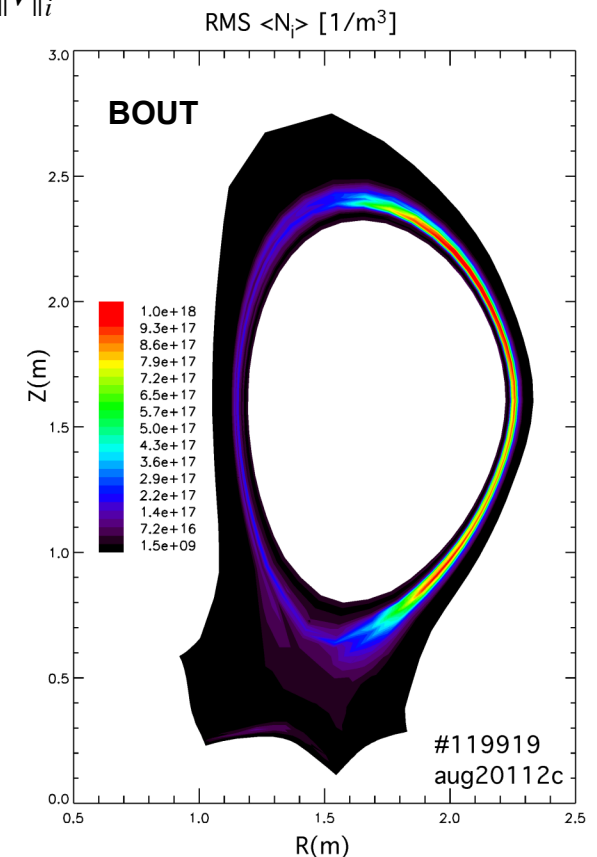
$$\frac{\partial V_{\parallel i}}{\partial t} + V_E \cdot \nabla V_{\parallel i} = -\frac{1}{N_i M_i} \nabla_{\parallel} P$$

$$\mathbf{E} = -\frac{1}{c} \frac{\partial}{\partial t} \mathbf{A}_{\parallel} - \nabla \phi, \quad -\nabla_{\perp}^2 \mathbf{A}_{\parallel} = \frac{4\pi}{c} \mathbf{j}_{\parallel}, \quad \mathbf{B} = \nabla \times \mathbf{A}_{\parallel} + \mathbf{B}_0$$

$$\varpi = \nabla \cdot (e Z_i N_i \nabla \phi) \approx e Z_i N_i \nabla^2 \phi \quad \nabla_{\parallel} \approx \mathbf{b}_0 \cdot \nabla$$

- Electromagnetic with $\nabla_{\parallel} \approx \mathbf{b}_0 \cdot \nabla$
- Finite-difference equations
- Implicit time integration with PVODE
- Quasi-ballooning with zero-gradient radial bdy conditions

Distribution of $\langle \delta N_i \rangle$ in saturated turbulence



Resistive Ballooning Simulations with BOUT -- Odd-even Numerical Mode Can Be Controlled with Normalized Diffusive Damping in Poloidal Angle

- Control the odd-even mode with $\partial/\partial t \rightarrow \partial/\partial t + \nu^*(k_\theta)$ in the vorticity and ion density eqns with diffusion operator in poloidal angle and normalized coeff.:

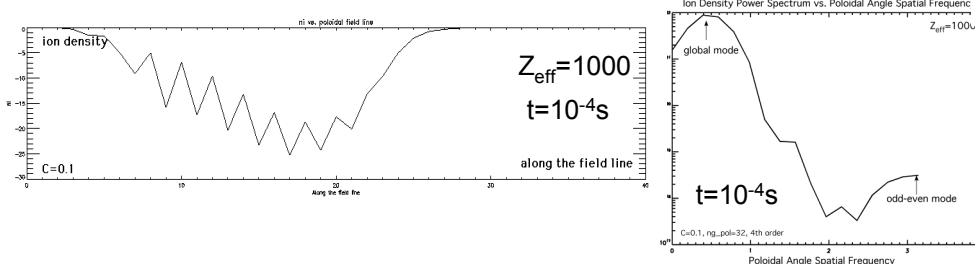
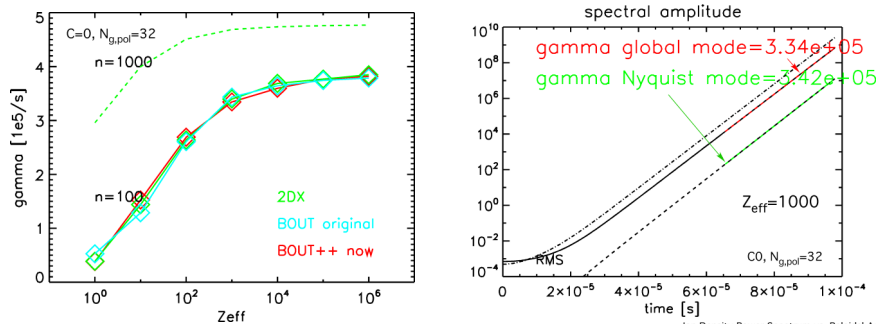
$$\nu^*(k_\theta) = \frac{C}{\Delta t} \left\{ -(\Delta\theta/2)^2 D_\theta^2, (\Delta\theta/2)^4 D_\theta^4 \right\} \rightarrow \frac{C}{\Delta t} \left\{ \sin(k_\theta \Delta\theta/2)^2, \sin(k_\theta \Delta\theta/2)^4 \right\}$$

- Damping of the odd-even mode is proportional to normalized coefficient C

C=0

$n_{g,pol}=32$ 4th order

Odd-even mode evident

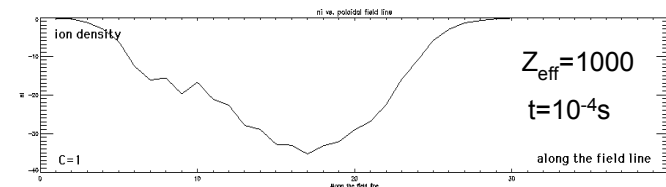
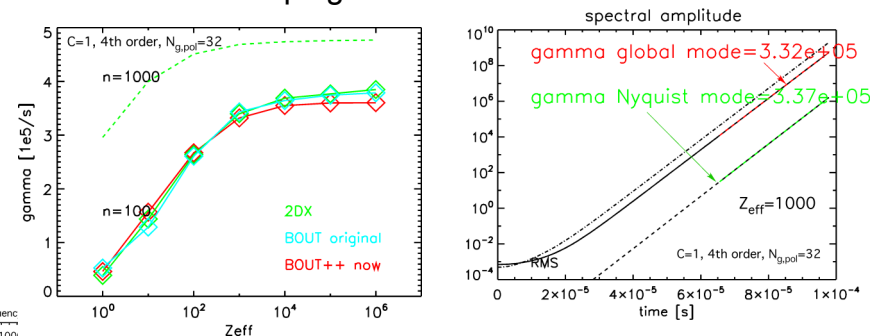


$$A(Nyquist)/A(global) \sim (\Delta x_\parallel^3) (\Delta x_\parallel/2L_\parallel)^n, \quad n = 2, 4$$

C=1

$n_{g,pol}=32$ 4th order

Damping of odd-even mode



- Note: Staggered grid for ∇_\parallel representation resolves problem with ∇_\parallel^2 finite-difference stencil & also removes odd-even mode

Case #1: BOUT06 produces expected ballooning-like turbulence in full DIII-D X-point geometry

- Consider the following simplified equation set in the BOUT06 framework:

$$\frac{\partial N_i}{\partial t} + (V_E + V_{\parallel}) \cdot \nabla N_i = \left(\frac{2c}{eB} \right) b_0 \times \kappa \cdot (\nabla P_e - N_i e \nabla \phi) + \nabla_{\parallel} (j_{\parallel} / e) - N_i \nabla_{\parallel} V_{\parallel i}$$

$$\frac{\partial \varpi}{\partial t} + V_E \cdot \nabla \varpi = 2\omega_{ci} b_0 \times \kappa \cdot \nabla P + N_i Z_i e \frac{4\pi V_A^2}{c^2} \nabla_{\parallel} j_{\parallel}$$

$$\frac{\partial V_{\parallel e}}{\partial t} = -\frac{e}{m_e} E_{\parallel} - \frac{1}{Nm_e} (T_e \nabla_{\parallel} N_i) + 0.51 \nu_{ei} j_{\parallel}$$

$$\frac{\partial V_{\parallel i}}{\partial t} + V_E \cdot \nabla V_{\parallel i} = -\frac{1}{N_i M_i} \nabla_{\parallel} P$$

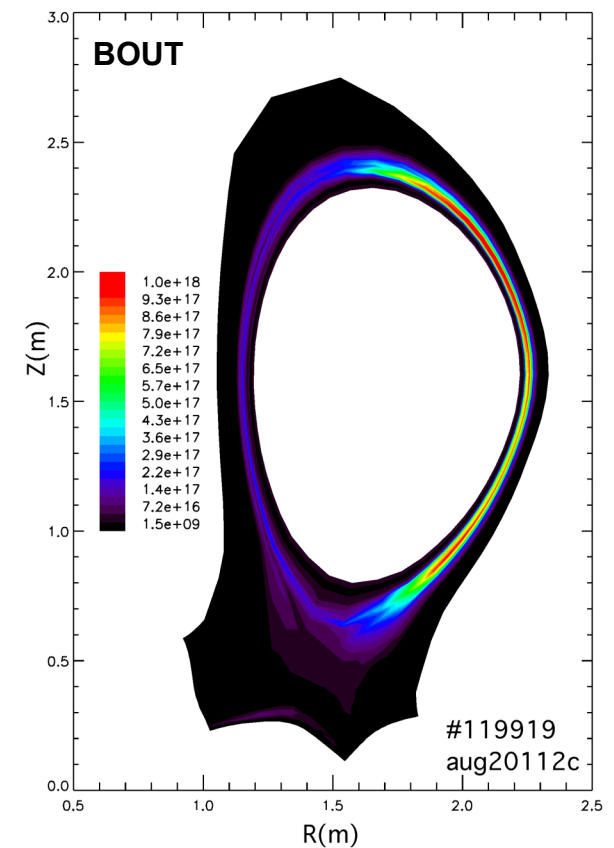
$$\mathbf{E} = -\frac{1}{c} \frac{\partial}{\partial t} \mathbf{A}_{\parallel} - \nabla \phi, \quad -\nabla_{\perp}^2 \mathbf{A}_{\parallel} = \frac{4\pi}{c} \mathbf{j}_{\parallel}, \quad \mathbf{B} = \nabla \times \mathbf{A}_{\parallel} + \mathbf{B}_0$$

$$\varpi = \nabla \cdot (e Z_i N_i \nabla \phi) \approx e Z_i N_i \nabla^2 \phi \quad \nabla_{\parallel} \approx \mathbf{b}_0 \cdot \nabla$$

- Electromagnetic with $\nabla_{\parallel} \approx \mathbf{b}_0 \cdot \nabla$
- Actual DIII-D geometry
- DIII-D - like fixed background profiles for shot 119919
- No T_e fluctuations

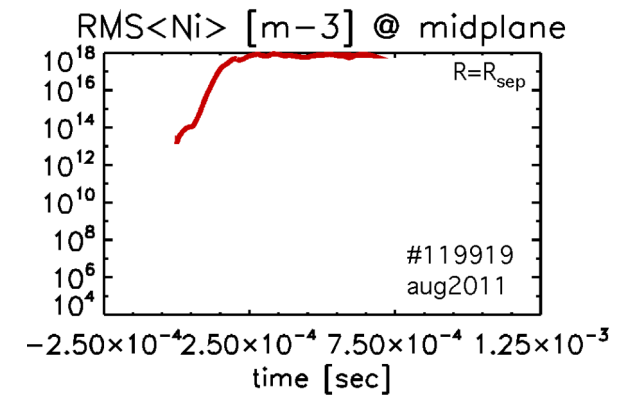
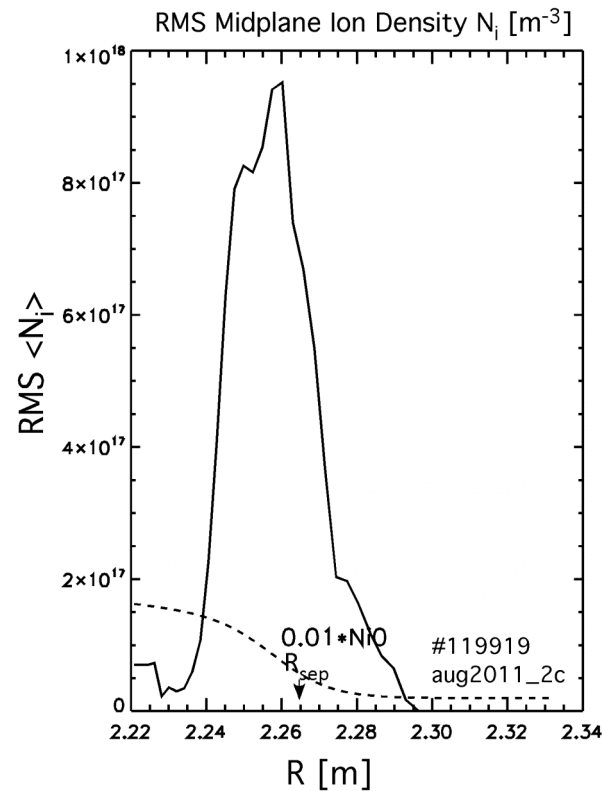
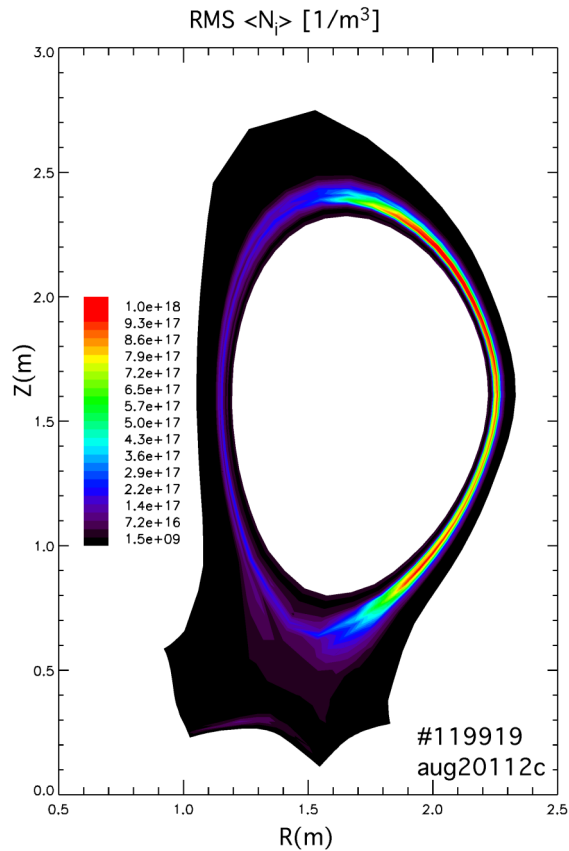
**Distribution of $\langle \delta N_i \rangle$
in saturated turbulence**

RMS $\langle N_i \rangle$ [1/m³]



Time-averaged ion density fluctuations in the midplane saturate at $\sim 10\%$ and peak near R_{sep}

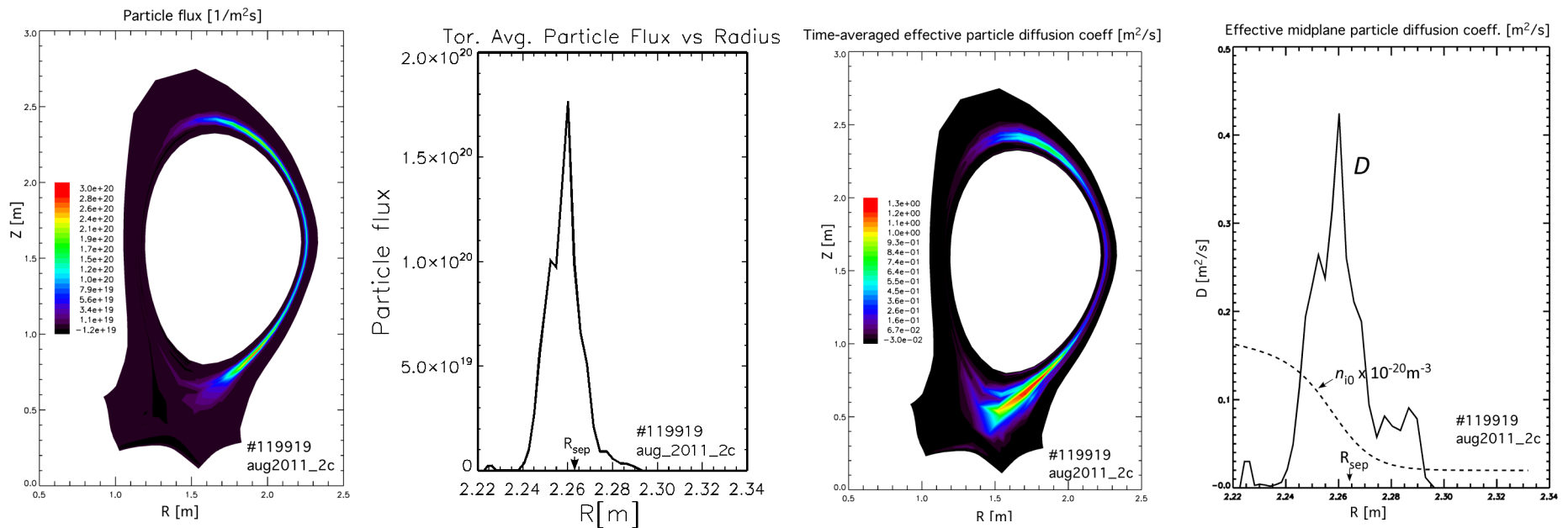
BOUT



- No T_e fluctuations

Time-averaged ion particle diffusion coefficient saturates at $O(0.4)$ m²/s in the midplane and peaks near R_{sep}

BOUT



- No T_e fluctuations
- In this model with no temperature fluctuations and if $\nabla \ln(T_{eq}) = \nabla \ln(n_{eq})$, then $\chi_{conv} \approx (3/2)D$

Case #2: Include Advection of Temperature T_e in BOUT06 Equations for Resistive Ballooning

- Consider the following simplified equation set in the BOUT06 framework:

$$\frac{\partial N_i}{\partial t} + (V_E + V_{\parallel}) \cdot \nabla N_i = \left(\frac{2c}{eB} \right) b_0 \times \kappa \cdot (\nabla P_e - N_i e \nabla \phi) + \nabla_{\parallel} (j_{\parallel} / e) - N_i \nabla_{\parallel} V_{\parallel i} \quad \text{RMS} \langle T_e \rangle \text{ [eV]}$$

$$\frac{\partial \varpi}{\partial t} + V_E \cdot \nabla \varpi = 2\omega_{ci} b_0 \times \kappa \cdot \nabla P + N_i Z_i e \frac{4\pi V_A^2}{c^2} \nabla_{\parallel} j_{\parallel}$$

$$\frac{\partial V_{\parallel e}}{\partial t} = -\frac{e}{m_e} E_{\parallel} - \frac{1}{Nm_e} (T_e \nabla_{\parallel} N_i) + 0.51 \nu_{ei} j_{\parallel}$$

$$\frac{\partial V_{\parallel i}}{\partial t} + V_E \cdot \nabla V_{\parallel i} = -\frac{1}{N_i M_i} \nabla_{\parallel} P$$

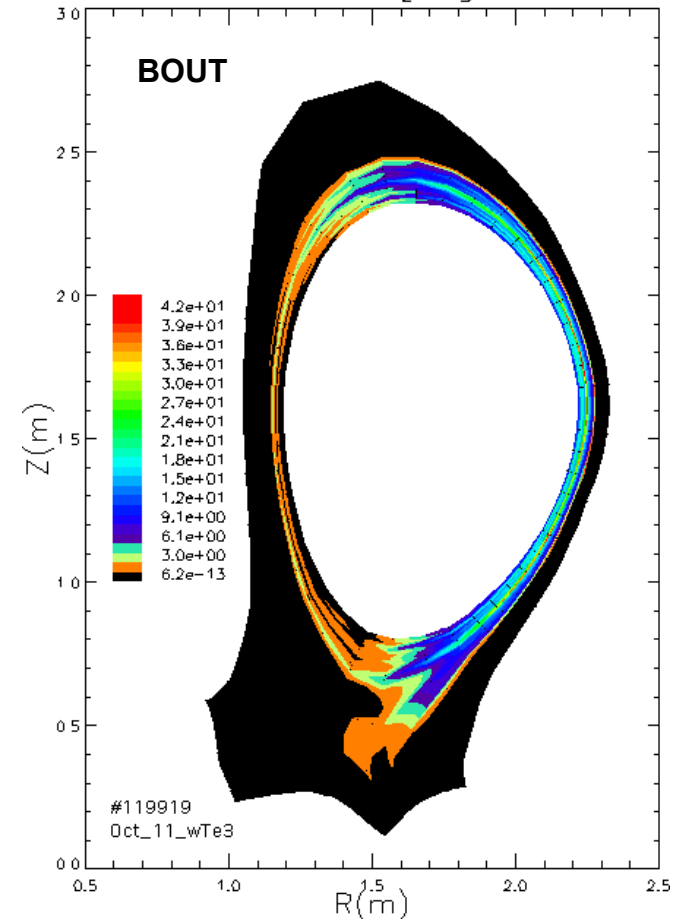
$$\frac{\partial T_e}{\partial t} + V_E \cdot \nabla T_e = 0$$

$$\mathbf{E} = -\frac{1}{c} \frac{\partial}{\partial t} \mathbf{A}_{\parallel} - \nabla \phi, \quad -\nabla_{\perp}^2 \mathbf{A}_{\parallel} = \frac{4\pi}{c} \mathbf{j}_{\parallel}, \quad \mathbf{B} = \nabla \times \mathbf{A}_{\parallel} + \mathbf{B}_0$$

$$\varpi = \nabla \cdot (e Z_i N_i \nabla \phi) \approx e Z_i N_i \nabla^2 \phi \quad \nabla_{\parallel} \approx \mathbf{b}_0 \cdot \nabla$$

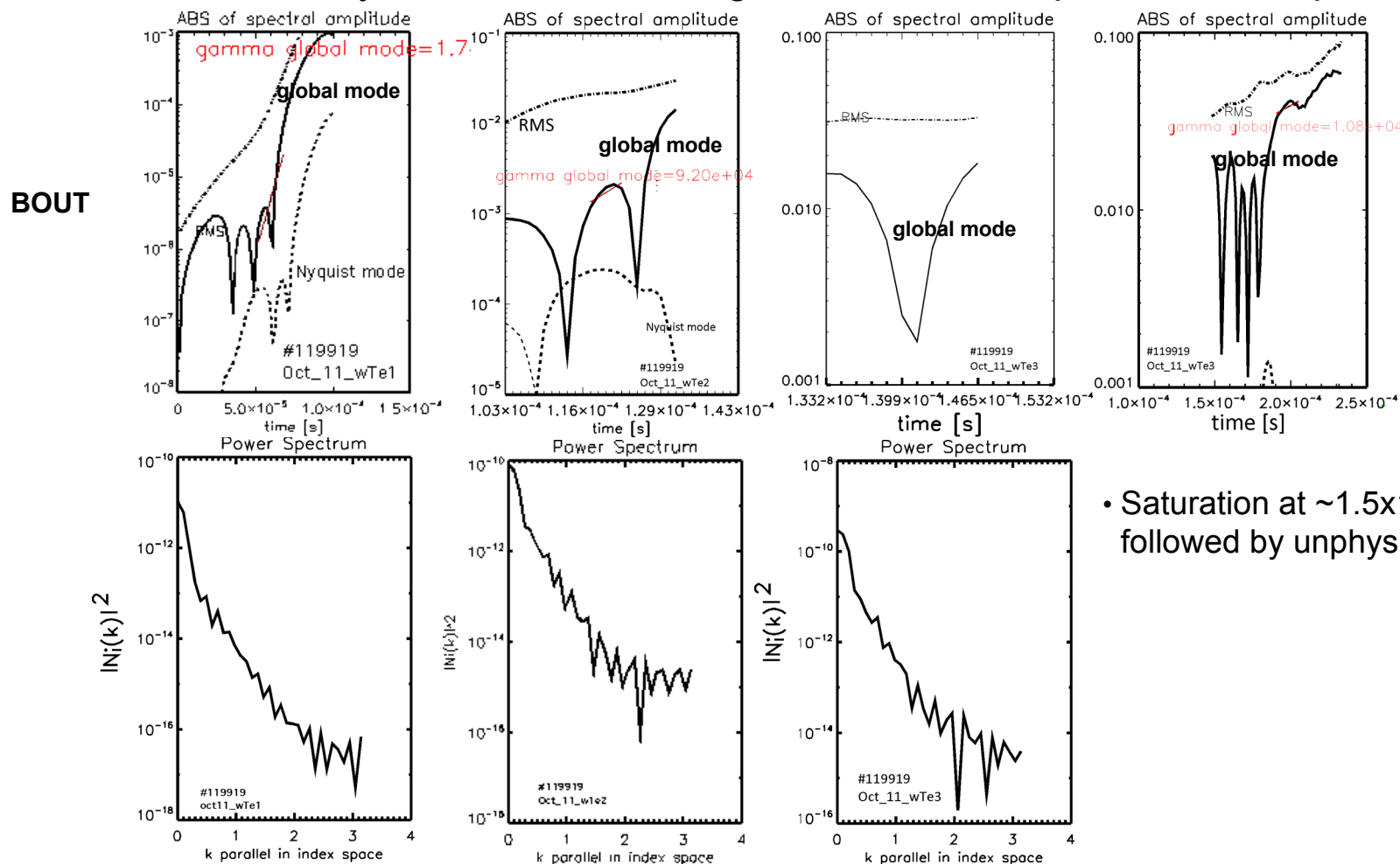
- Electromagnetic with $\nabla_{\parallel} \approx \mathbf{b}_0 \cdot \nabla$
- Actual DIII-D geometry
- DIII-D - like fixed background profiles for shot 119919
- Includes T_e fluctuations

B. Cohen, et al., APS DPP 2011



BOUT-06 produces saturated turbulence for DIII-D geometry with T_e fluctuations

- Evolution of density fluctuations leading to saturated amplitudes and spectra



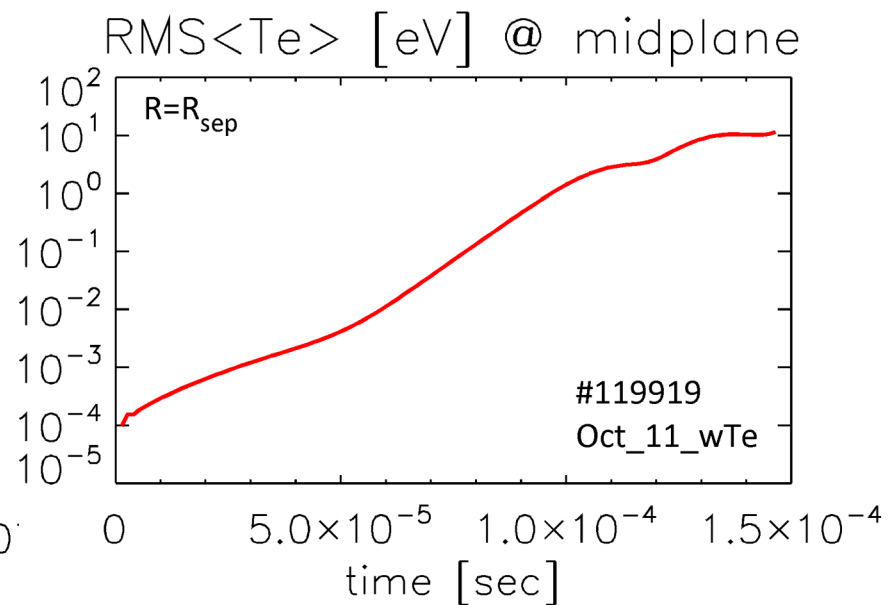
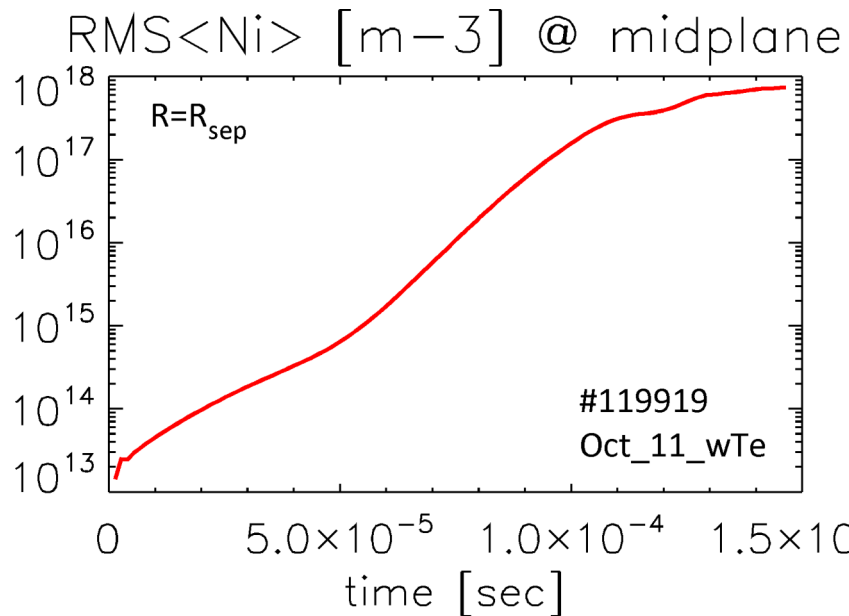
- Saturation at $\sim 1.5 \times 10^{-4}$ s followed by unphysical growth

- With T_e fluctuations

B. Cohen, et al., APS DPP 2011

Ion density and electron T_e fluctuations in the midplane saturate at $\sim 1.5 \times 10^{-4}$ sec

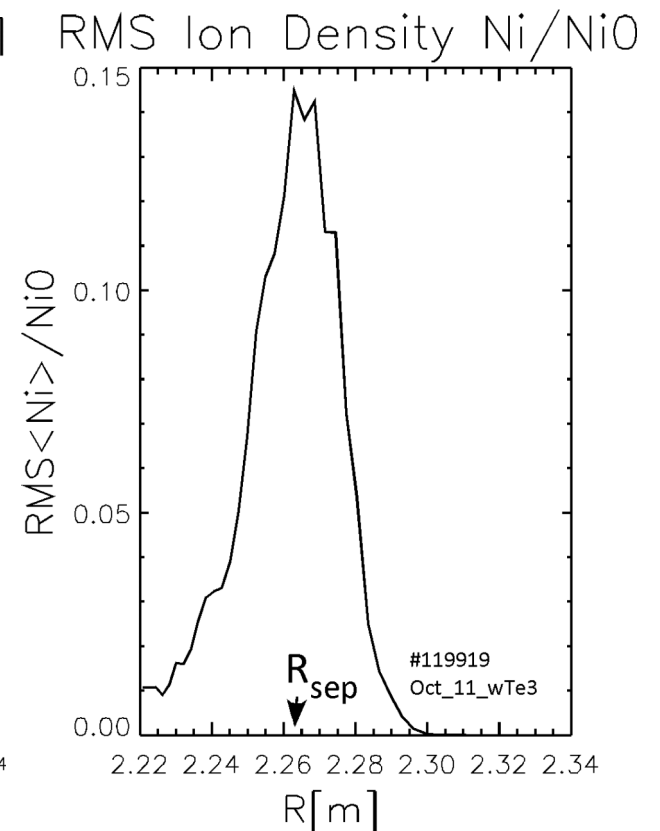
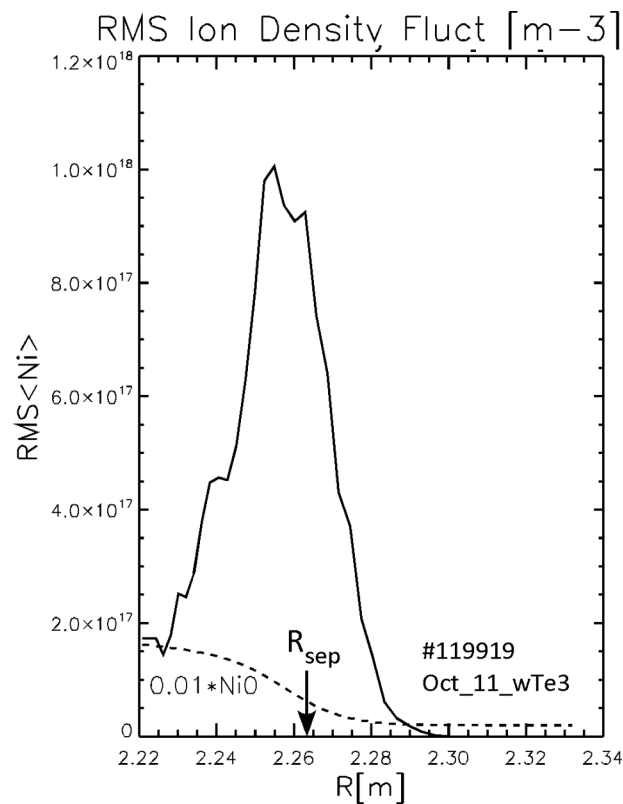
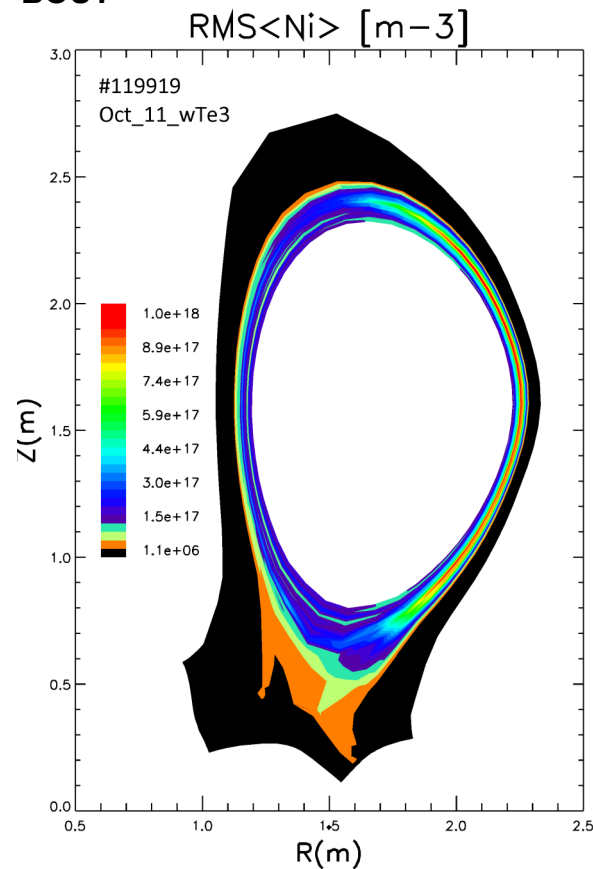
BOUT



- With T_e fluctuations

Time-averaged ion density fluctuations in the midplane saturate at $\sim 15\%$ relative amplitude and peak near R_{sep}

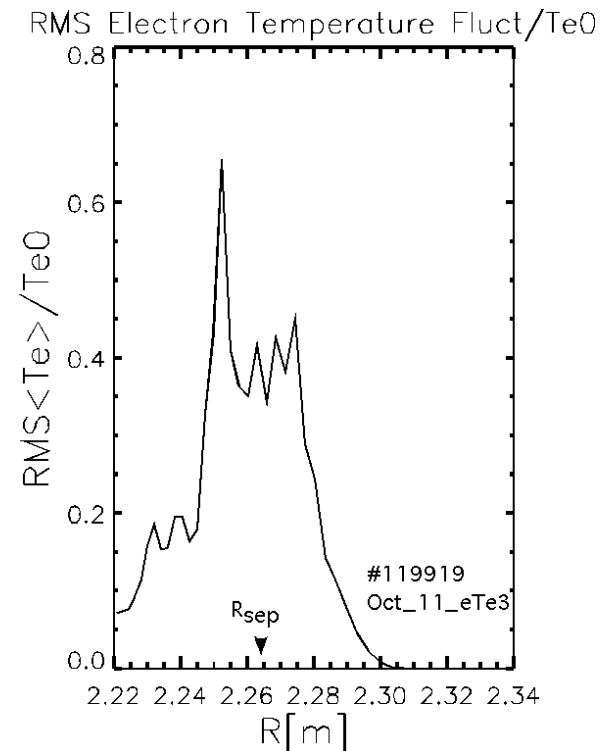
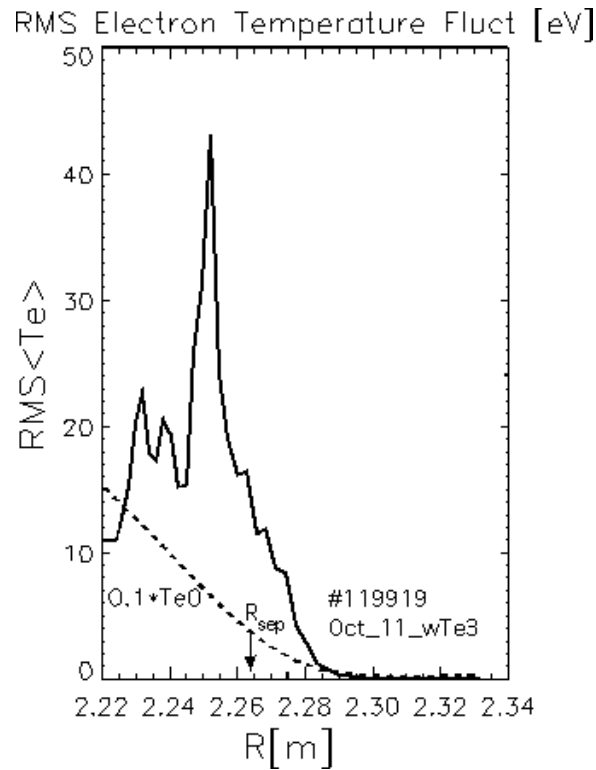
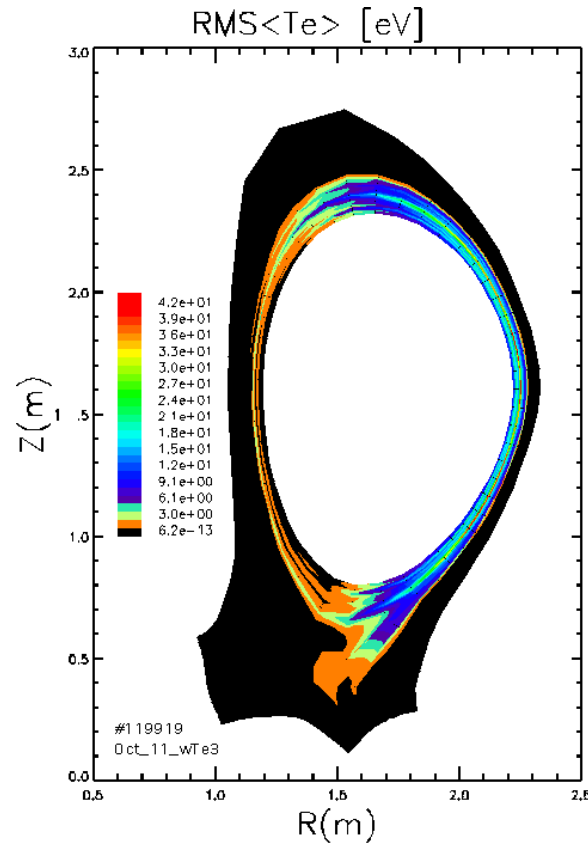
BOUT



- With T_e fluctuations

Time-averaged T_e fluctuations in the midplane saturate at ~40-60% relative amplitude and peak near R_{sep}

BOUT

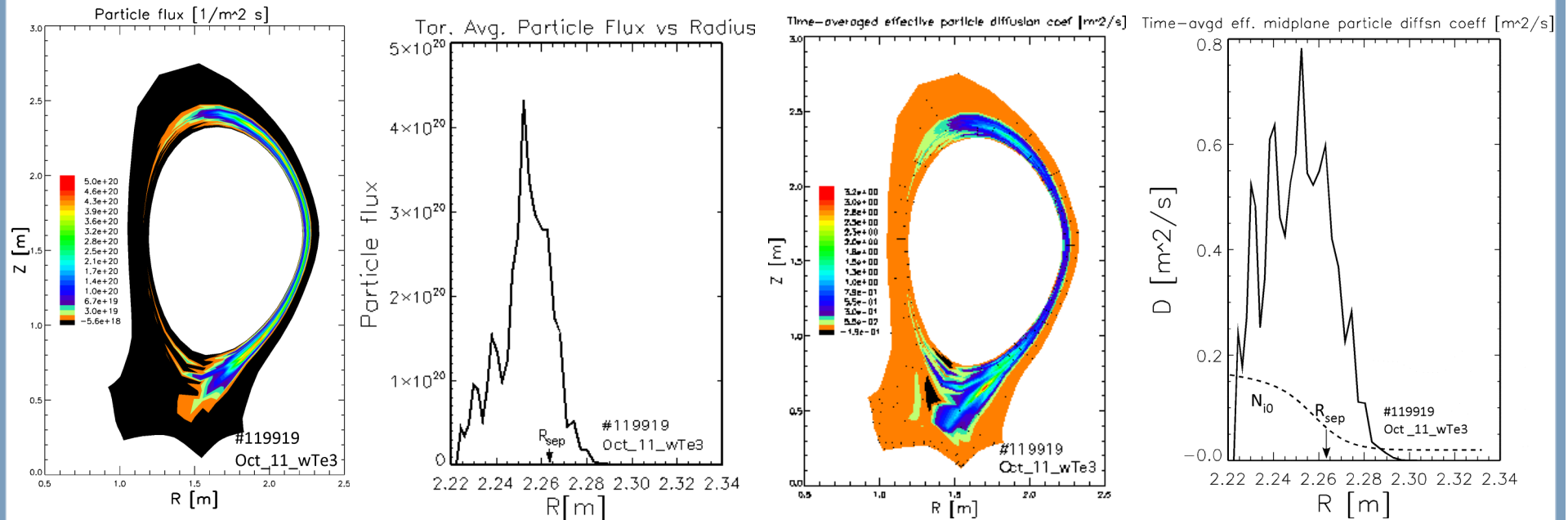


- With T_e fluctuations

B. Cohen, et al., APS DPP 2011

Time-averaged ion particle diffusion coefficient in the midplane saturates at $O(1) \text{ m}^2/\text{s}$ and peaks near R_{sep}

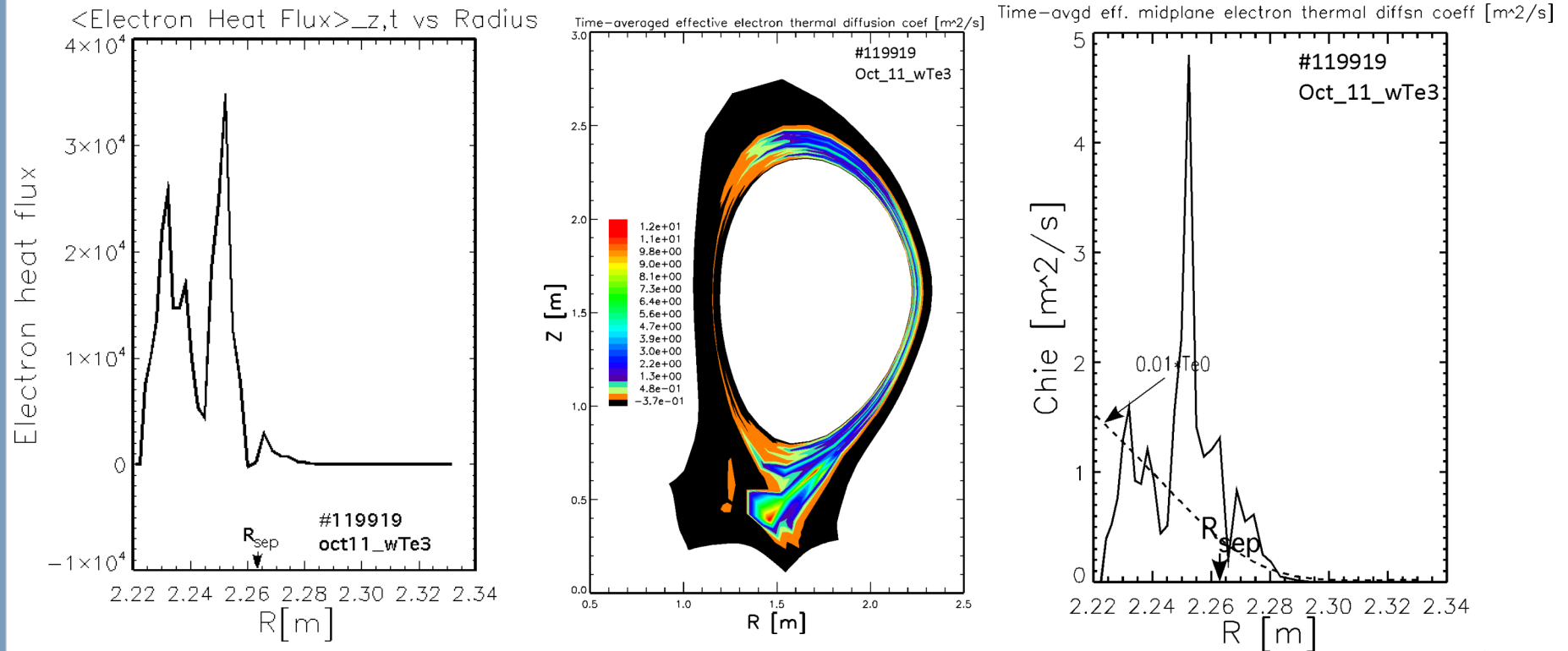
BOUT



- With T_e fluctuations

Time-averaged electron thermal diffusion coefficient in the midplane saturates at 1-5 m²/s and peaks near R_{sep}

- Bout with T_e fluctuations



Note : Here heat flux (conductive) = $N_0 \langle \delta \tilde{v}_r \delta T_e \rangle_{tor,t}$, and $\chi_e = -N_0 \langle \delta \tilde{v}_r \delta T_e \rangle_{tor,t} / N_0 \nabla T_{e0}$

Case #3: Include Advection of T_e in BOUT06 Equations for Resistive Ballooning with Parallel Electron Thermal Conduction

- Consider the following simplified equation set in the BOUT06 framework:

$$\frac{\partial N_i}{\partial t} + (V_E + V_{\parallel}) \cdot \nabla N_i = \left(\frac{2c}{eB} \right) b_0 \times \kappa \cdot (\nabla P_e - N_i e \nabla \varphi) + \nabla_{\parallel} (j_{\parallel} / e) - N_i \nabla_{\parallel} V_{\parallel i}$$

$$\frac{\partial \varpi}{\partial t} + V_E \cdot \nabla \varpi = 2\omega_{ci} b_0 \times \kappa \cdot \nabla P + N_i Z_i e \frac{4\pi V_A^2}{c^2} \nabla_{\parallel} j_{\parallel}$$

$$\frac{\partial V_{\parallel e}}{\partial t} = -\frac{e}{m_e} E_{\parallel} - \frac{1}{Nm_e} (T_e \nabla_{\parallel} N_i) + 0.51 \nu_{ei} j_{\parallel}$$

$$\frac{\partial V_{\parallel i}}{\partial t} + V_E \cdot \nabla V_{\parallel i} = -\frac{1}{N_i M_i} \nabla_{\parallel} P$$

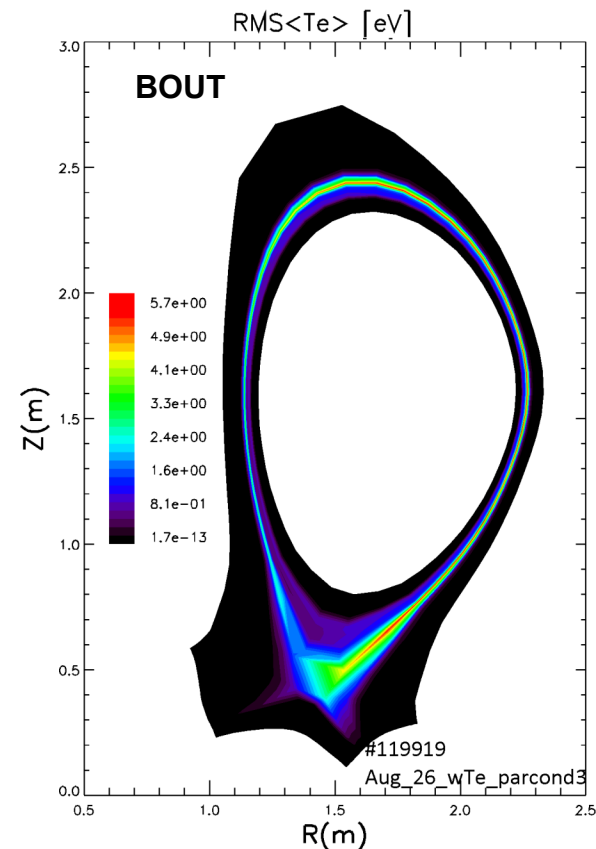
$$\frac{\partial T_e}{\partial t} + V_E \cdot \nabla T_e = \frac{2}{3N_0} \nabla \cdot (\kappa_{\parallel}^e \nabla T_e), \quad \kappa_{\parallel}^e = 3.2 \frac{N_0 T_{e0} \tau_e}{m_e}$$

$$\mathbf{E} = -\frac{1}{c} \frac{\partial}{\partial t} \mathbf{A}_{\parallel} - \nabla \varphi, \quad -\nabla_{\perp}^2 \mathbf{A}_{\parallel} = \frac{4\pi}{c} \mathbf{j}_{\parallel}, \quad \mathbf{B} = \nabla \times \mathbf{A}_{\parallel} + \mathbf{B}_0$$

$$\varpi = \nabla \cdot (e Z_i N_i \nabla \varphi) \approx e Z_i N_i \nabla^2 \varphi \quad \nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla$$

- Electromagnetic with $\nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla$
- Actual DIII-D geometry
- DIII-D - like fixed background profiles for shot #119919
- Includes T_e fluctuations & parallel heat conduction

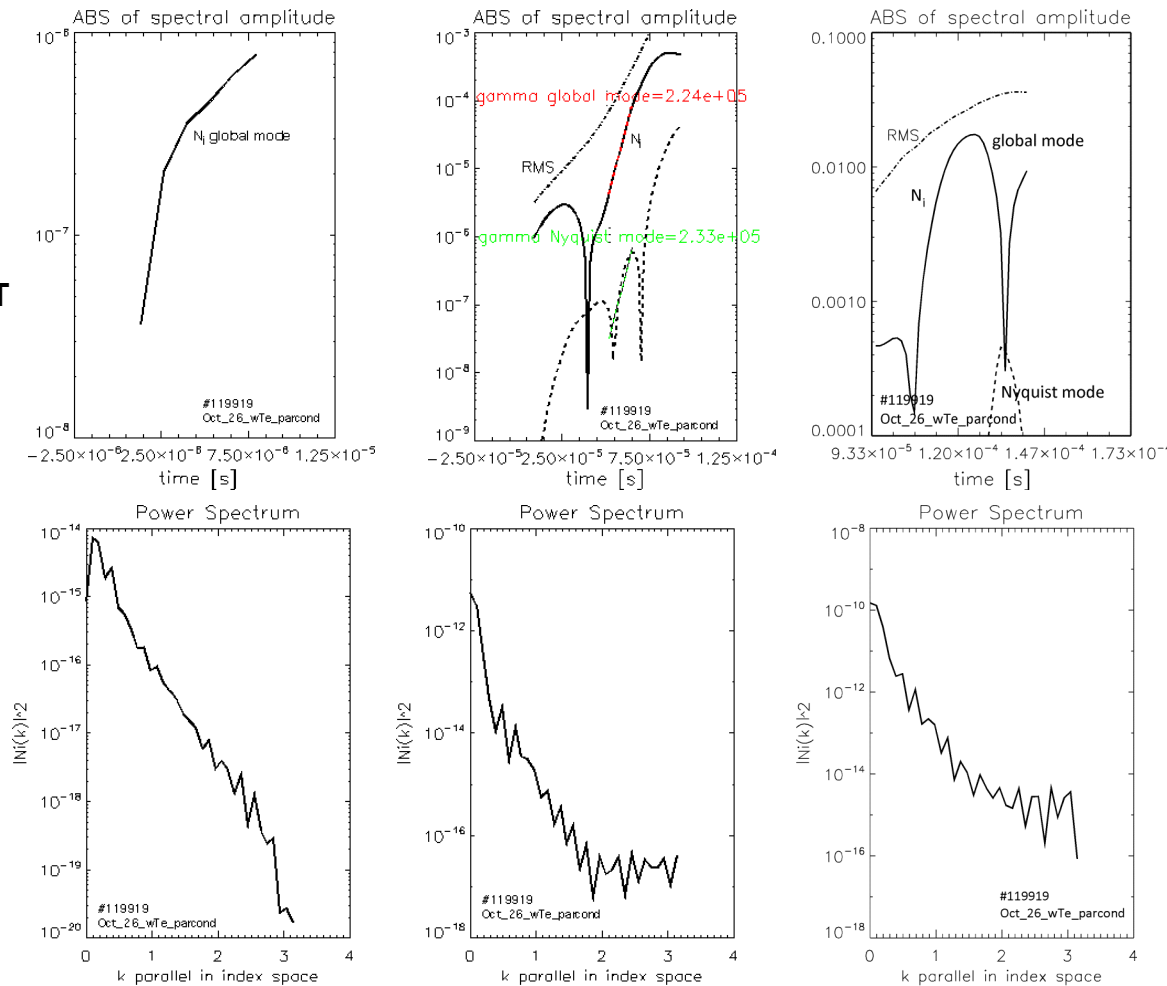
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BOUT-06 produces saturated turbulence for DIII-D geometry with T_e fluctuations and electron parallel thermal conduction

- Evolution of density fluctuations leading to saturated amplitudes and spectra

BOUT



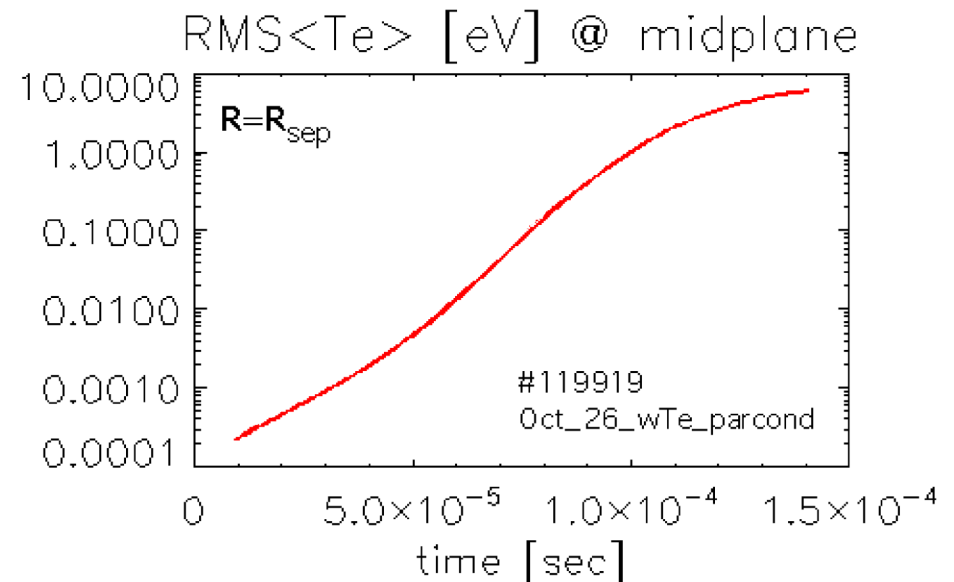
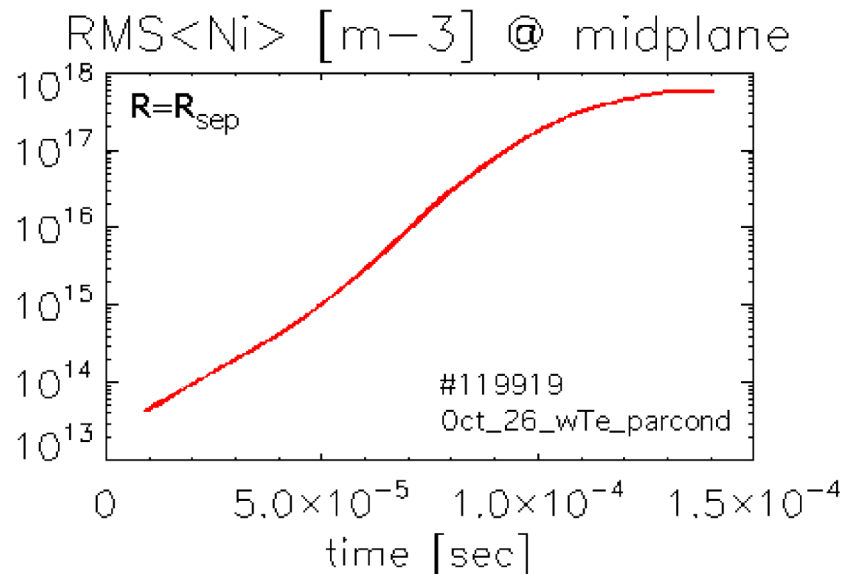
- Saturation at $\sim 1.5 \times 10^{-4}$ s

- With T_e fluctuations and electron parallel thermal conduction

B. Cohen, et al., APS DPP 2011

History of rms fluctuation amplitudes in midplane at separatrix with electron parallel thermal conduction

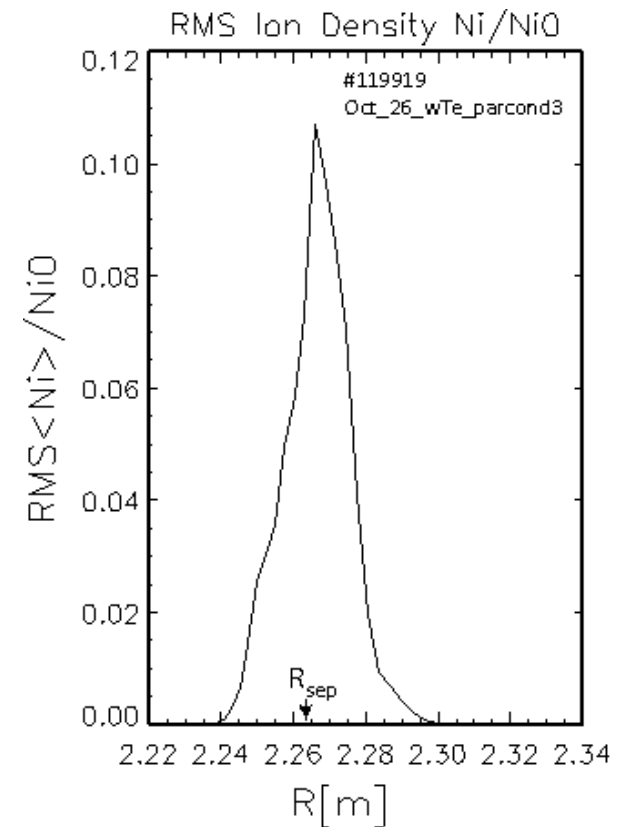
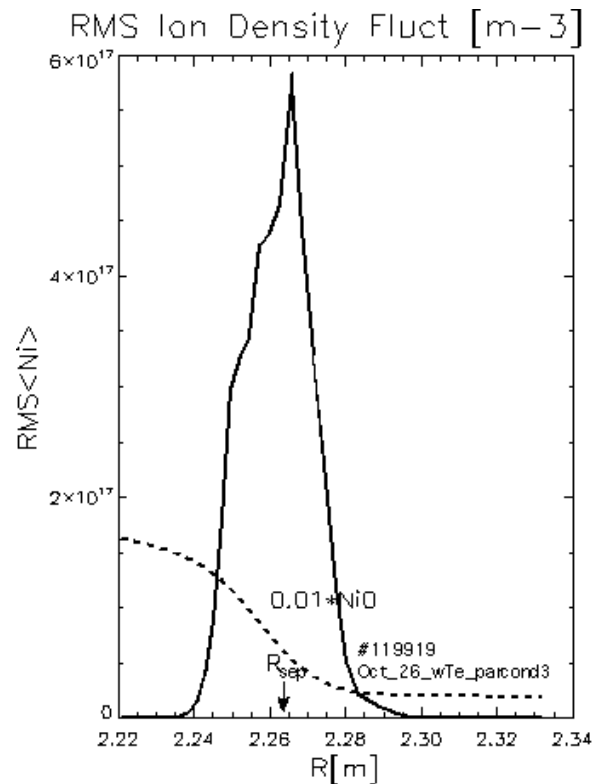
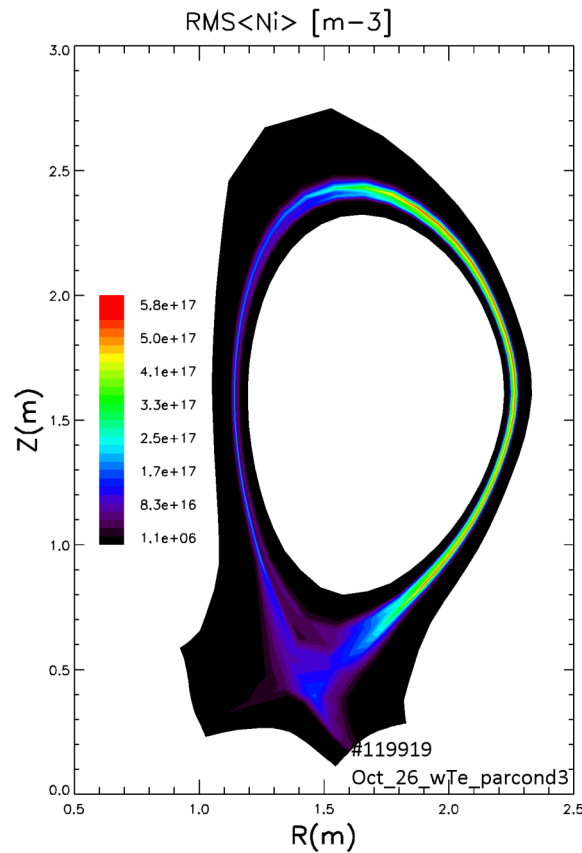
BOUT



- With T_e fluctuations and electron parallel thermal conduction

Time-averaged ion density fluctuations in the midplane saturate at $\sim 11\%$ and peak near R_{sep}

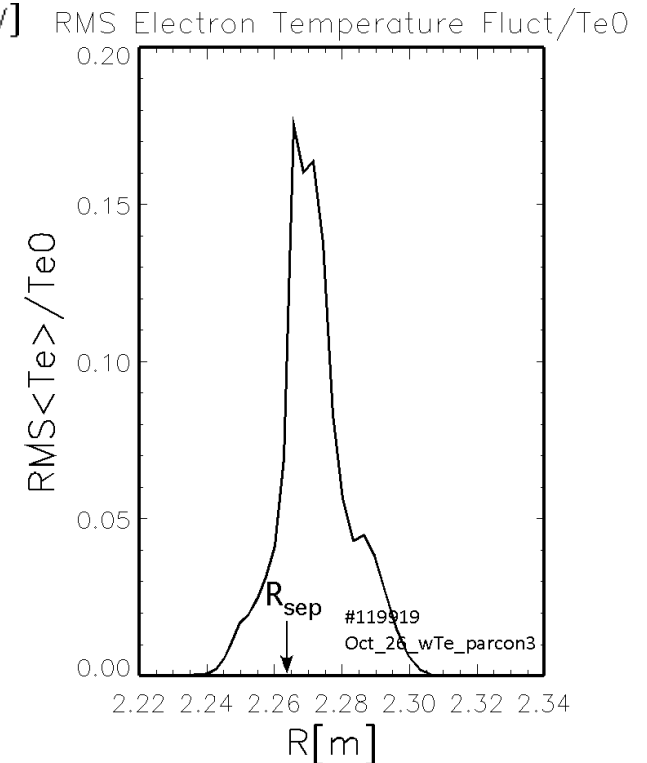
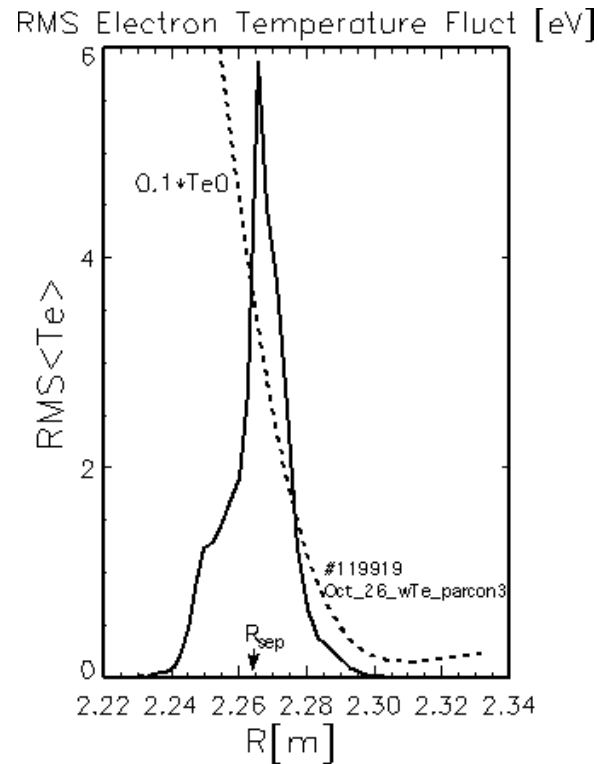
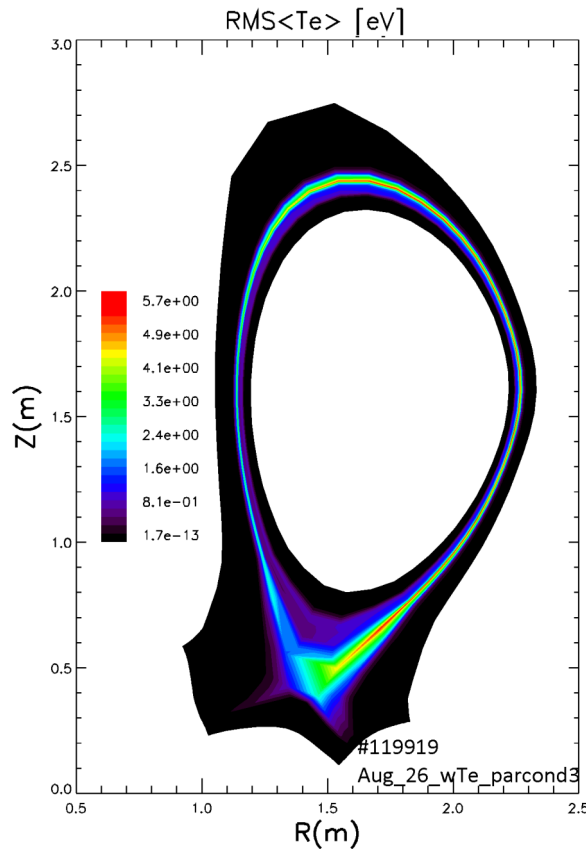
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- With T_e fluctuations and electron parallel thermal conduction

Time-averaged T_e fluctuations in the midplane peak near the R_{sep} and saturate at $\sim 18\%$ relative amplitude

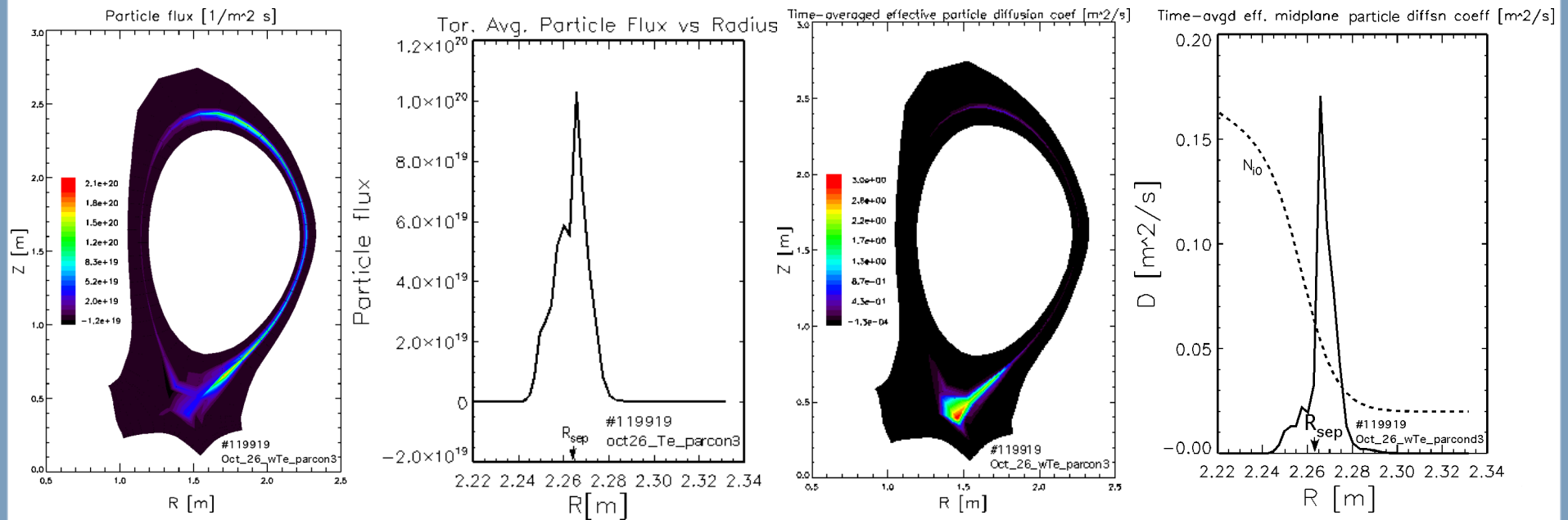
BOUT



- With T_e fluctuations and electron parallel thermal conduction

Time-averaged ion particle diffusion coefficient in the midplane saturates at $< 0.2 \text{ m}^2/\text{s}$ and peaks near R_{sep}

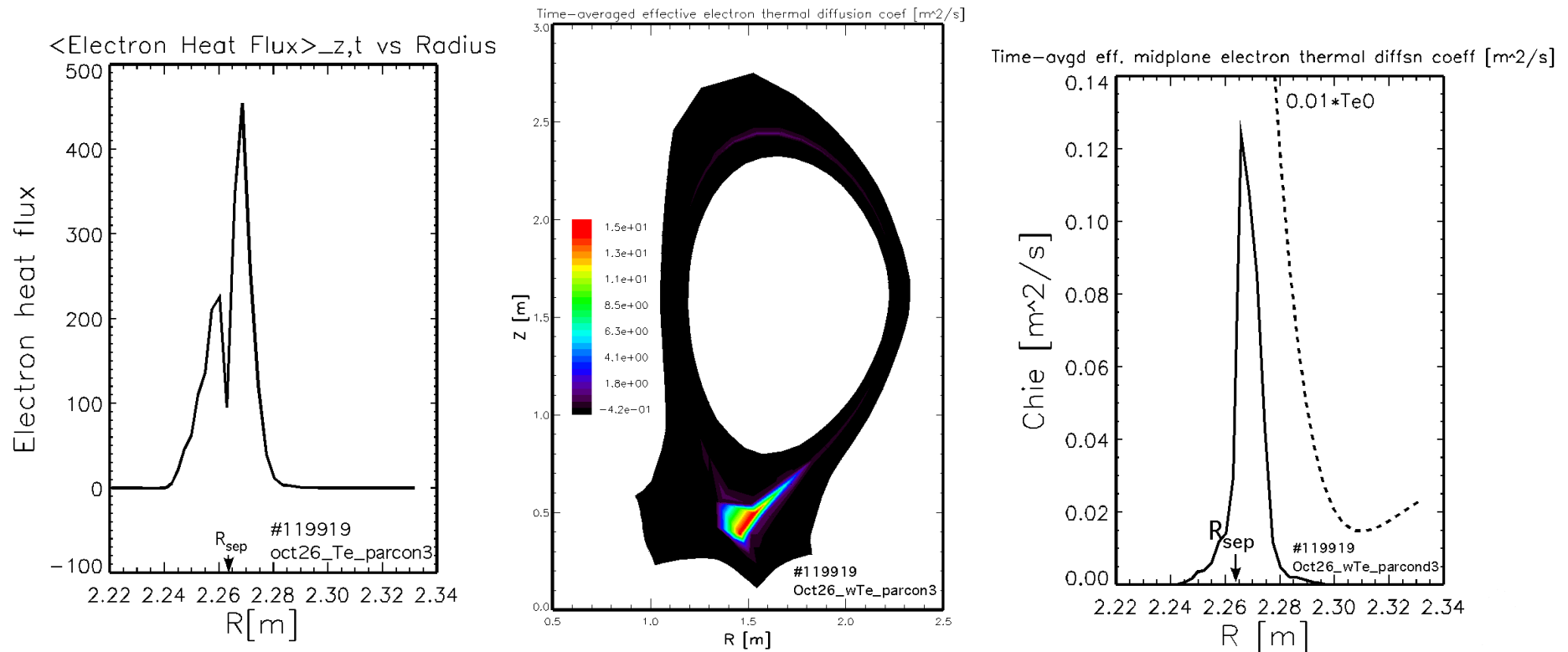
BOUT



- With T_e fluctuations and electron parallel thermal conduction

Time-averaged electron thermal diffusion coefficient in the midplane saturates at $\sim 0.1 \text{ m}^2/\text{s}$ and peaks near R_{sep}

BOUT



Note : Here heat flux (conductive) = $N_0 \langle \delta \tilde{v}_r \delta T_e \rangle_{\text{tor},t}$, and $\chi_e = -N_0 \langle \delta \tilde{v}_r \delta T_e \rangle_{\text{tor},t} / N_0 \nabla T_{e0}$

- With T_e fluctuations and electron parallel thermal conduction

Case #4: Include Advection of Temperature T_e in BOUT06 Equations for Resistive Ballooning with Magnetic Flutter

- Consider the following simplified equation set in the BOUT06 framework:

$$\frac{\partial N_i}{\partial t} + (V_E + V_{\parallel}) \cdot \nabla N_i = \left(\frac{2c}{eB} \right) b_0 \times \kappa \cdot (\nabla P_e - N_i e \nabla \varphi) + \nabla_{\parallel} (j_{\parallel} / e) - N_i \nabla_{\parallel} V_{\parallel i}$$

$$\frac{\partial \varpi}{\partial t} + V_E \cdot \nabla \varpi = 2\omega_{ci} b_0 \times \kappa \cdot \nabla P + N_i Z_i e \frac{4\pi V_A^2}{c^2} \nabla_{\parallel} j_{\parallel}$$

$$\frac{\partial V_{\parallel e}}{\partial t} = -\frac{e}{m_e} E_{\parallel} - \frac{1}{Nm_e} (T_e \nabla_{\parallel} N_i) + 0.51 \nu_{ei} j_{\parallel}$$

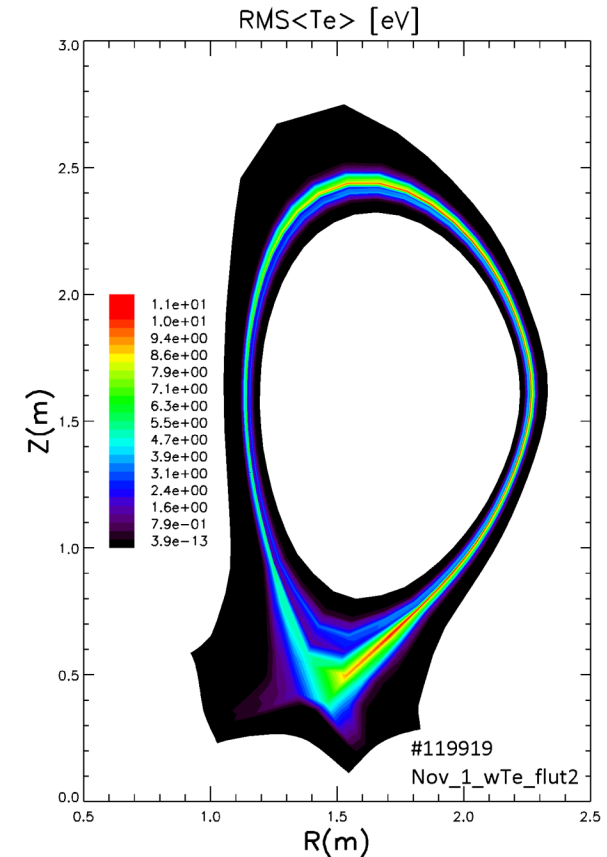
$$\frac{\partial V_{\parallel i}}{\partial t} + V_E \cdot \nabla V_{\parallel i} = -\frac{1}{N_i M_i} \nabla_{\parallel} P$$

$$\frac{\partial T_e}{\partial t} + V_E \cdot \nabla T_e = \frac{2}{3N_0} \nabla \cdot (\kappa_{\parallel}^e \nabla_{\parallel} T_e), \quad \kappa_{\parallel}^e = 3.2 \frac{n T_{e0} \tau_e}{m_e}$$

$$\mathbf{E} = -\frac{1}{c} \frac{\partial}{\partial t} \mathbf{A}_{\parallel} - \nabla \varphi, \quad -\nabla_{\perp}^2 \mathbf{A}_{\parallel} = \frac{4\pi}{c} \mathbf{j}_{\parallel}, \quad \mathbf{B} = \nabla \times \mathbf{A}_{\parallel} + \mathbf{B}_0$$

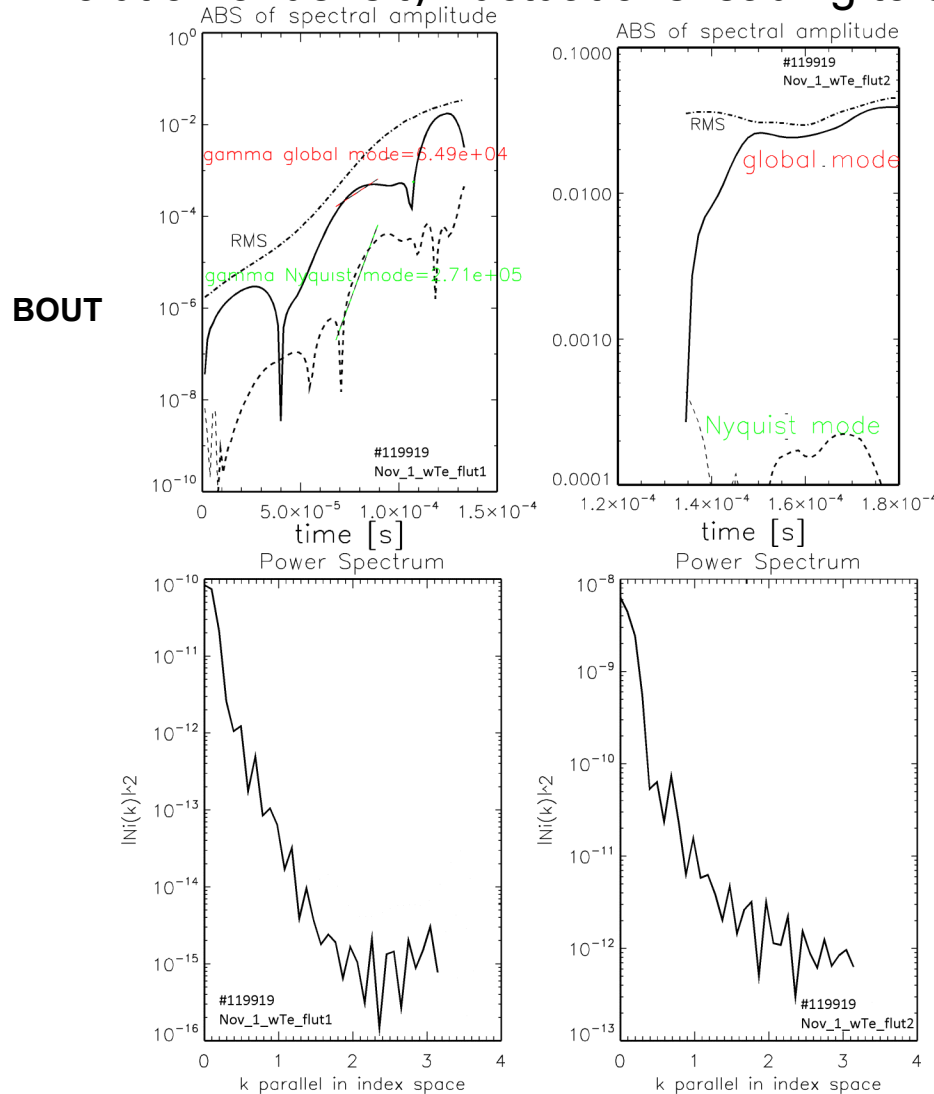
$$\varpi = \nabla \cdot (e Z_i N_i \nabla \varphi) \approx e Z_i N_i \nabla^2 \varphi \quad \nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$$

- Electromagnetic with $\nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$ in the vorticity eqn.
- Actual DIII-D geometry
- DIII-D - like fixed background profiles for shot 119919
- Includes T_e fluctuations and parallel heat conduction



BOUT-06 produces saturated turbulence for DIII-D geometry with δT_e , parallel thermal conduction, and magnetic flutter

- Evolution of density fluctuations leading to saturated amplitudes and spectra



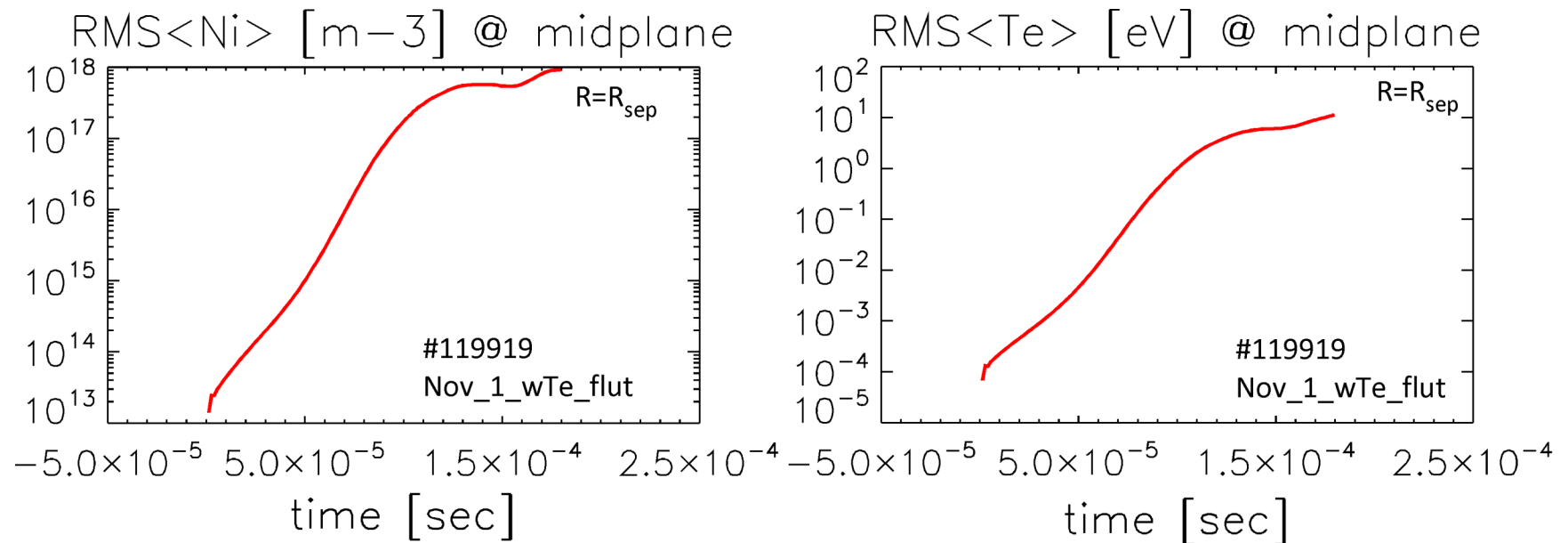
- Saturation at $\sim 1.5 \times 10^{-4}$ s

- With T_e fluctuations, electron parallel thermal conduction, and

$$\nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$$

History of rms fluctuation amplitudes in midplane at separatrix with electron parallel thermal conduction and magnetic flutter

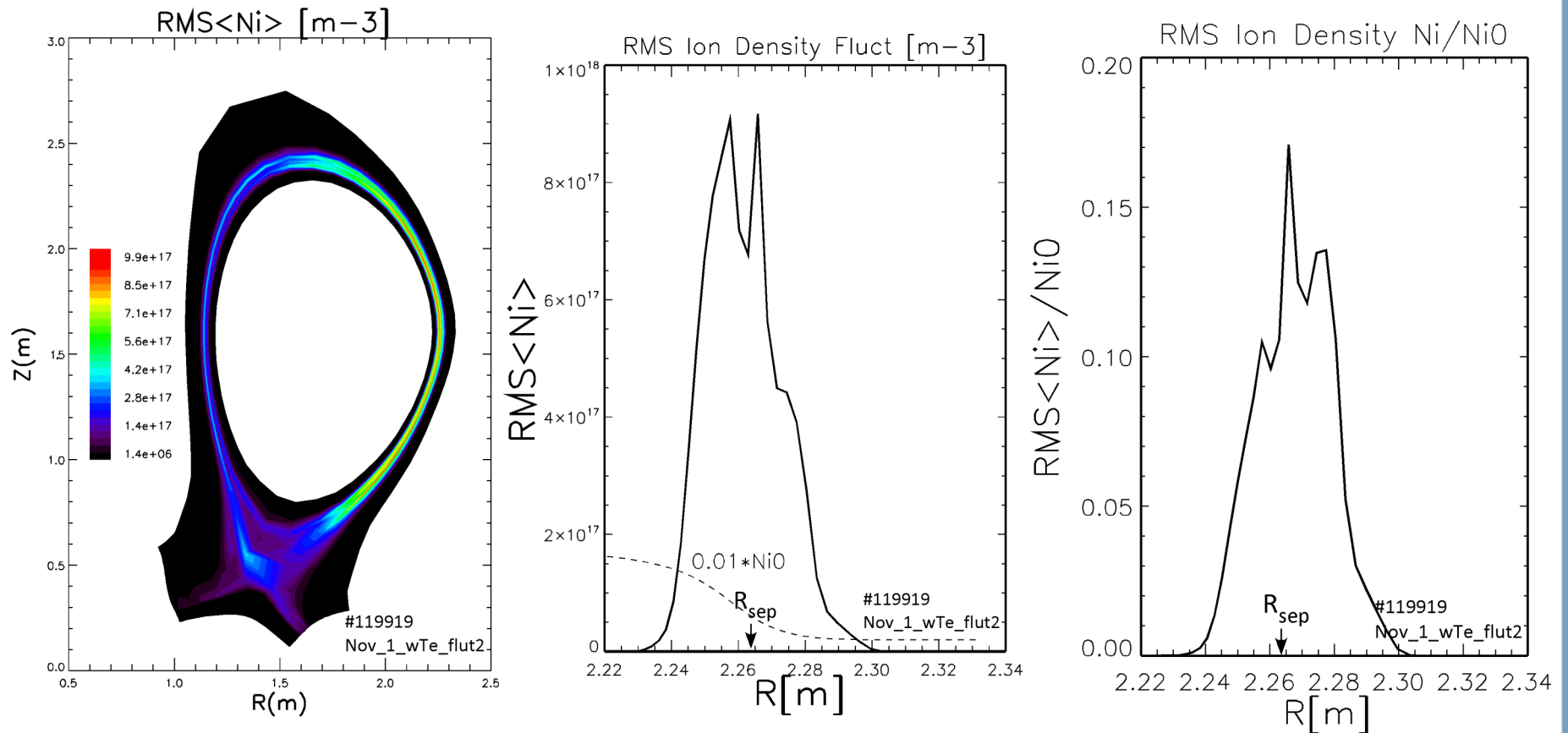
BOUT



- With T_e fluctuations, electron parallel thermal conduction, and $\nabla_{||} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$ in vorticity equation

Time-averaged ion density fluctuations in the midplane saturate at $\sim 10\text{-}15\%$ and peak near R_{sep}

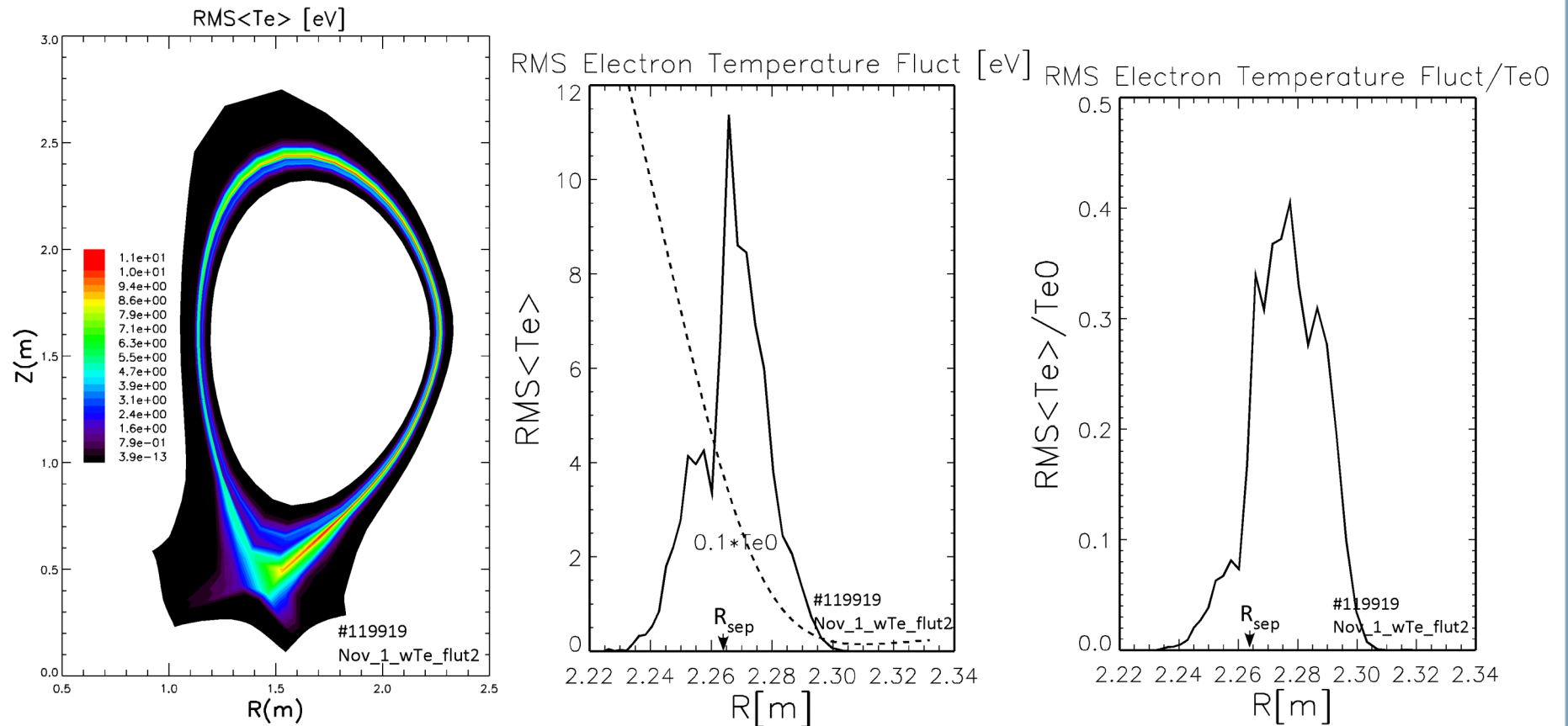
BOUT



- With T_e fluctuations, electron parallel thermal conduction, and $\nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$

Time-averaged T_e fluctuations in the midplane peak near the R_{sep} and saturate at ~25-40% relative amplitude

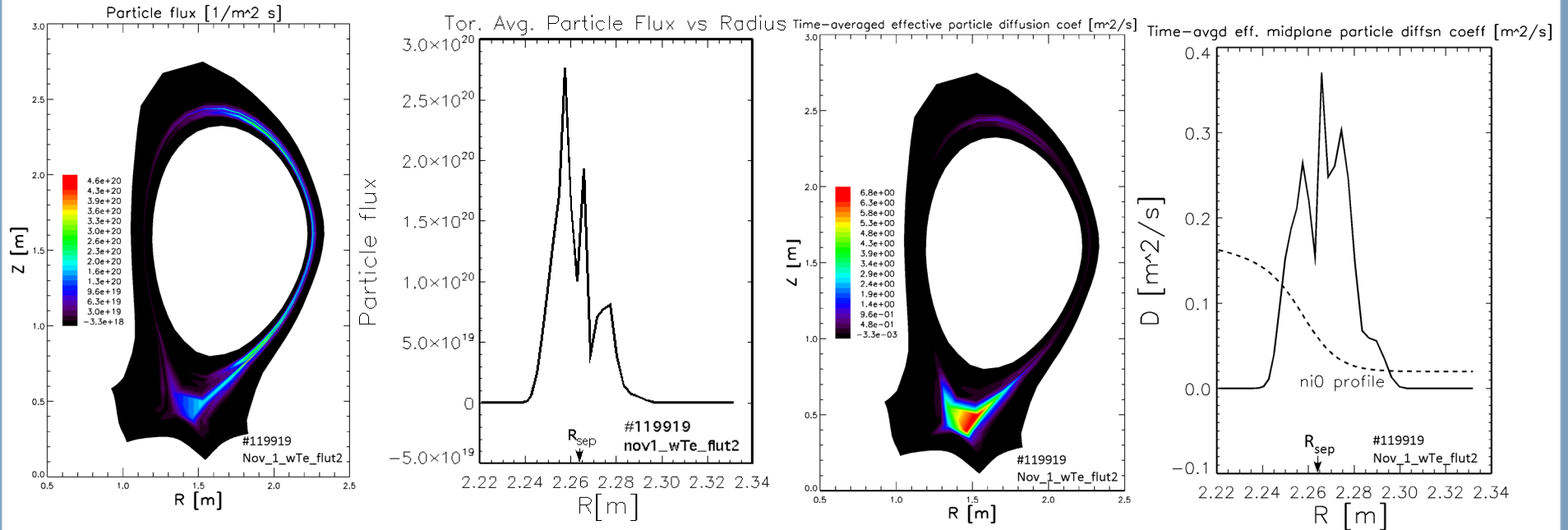
BOUT



- With T_e fluctuations, electron parallel thermal conduction, and $\nabla_{||} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$

Time-averaged ion particle diffusion coefficient in the midplane saturates at $< 0.3\text{-}0.4 \text{ m}^2/\text{s}$

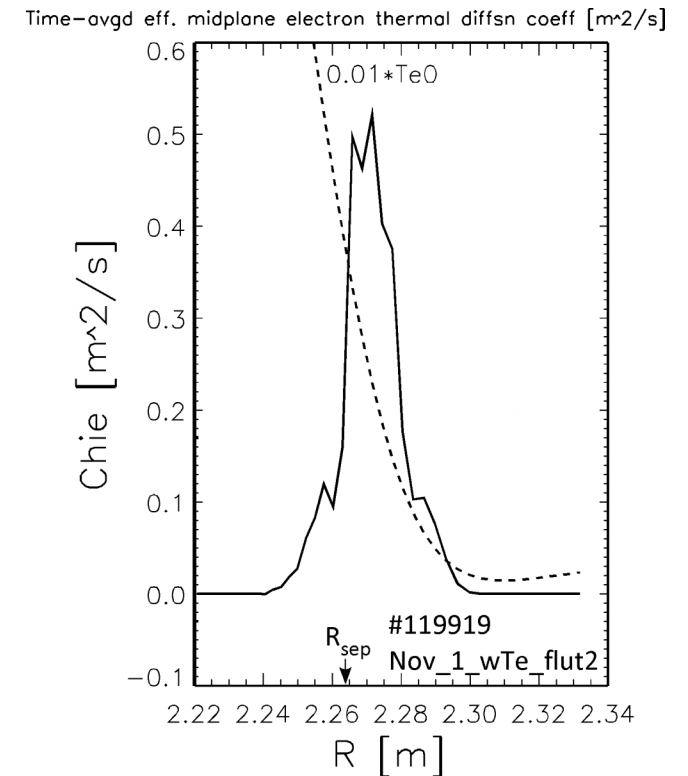
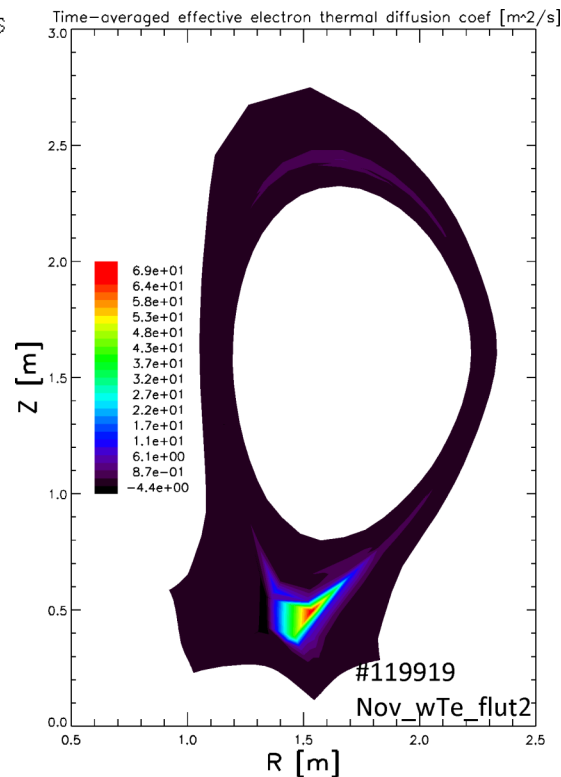
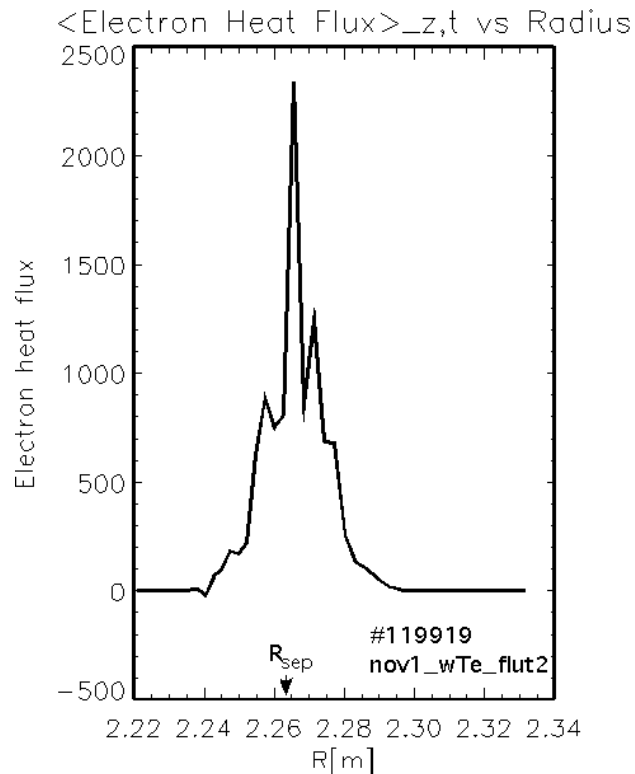
BOUT



- With T_e fluctuations, electron parallel thermal conduction, and $\nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$

Time-averaged electron thermal diffusion coefficient in the midplane saturates at $\sim 0.5 \text{ m}^2/\text{s}$

BOUT

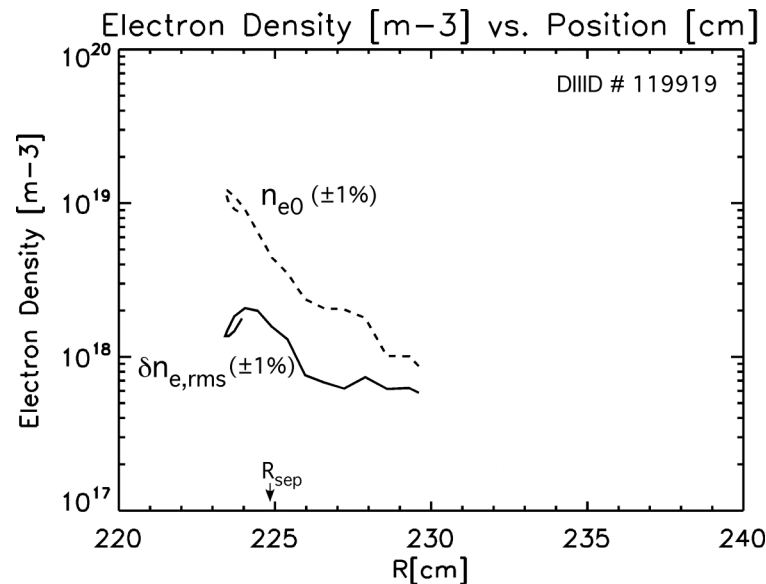


Note : Here heat flux (conductive) = $N_0 < \delta \tilde{v}_i \delta T_e >_{\text{tor},t}$, and $\chi_e = -N_0 < \delta \tilde{v}_i \delta T_e >_{\text{tor},t} / N_0 \nabla T_{e0}$

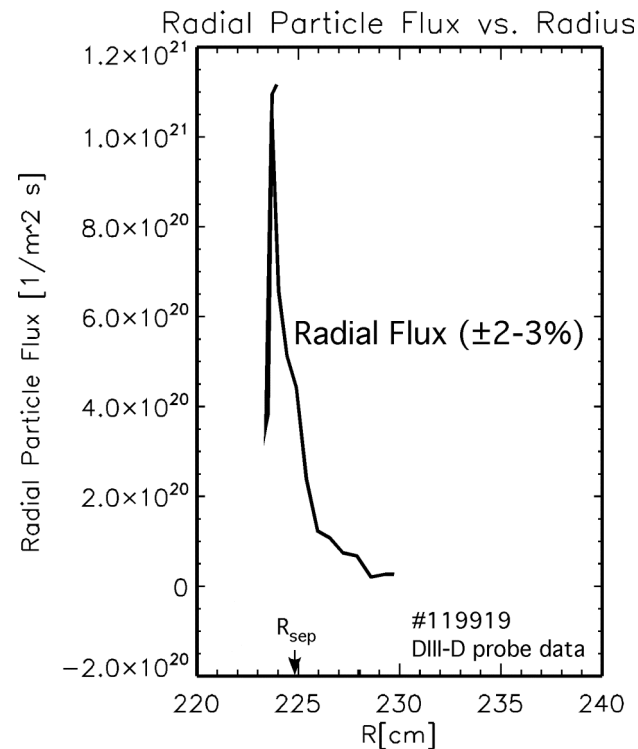
- With T_e fluctuations, electron parallel thermal conduction, and $\nabla_{\parallel} = \mathbf{b}_0 \cdot \nabla + \tilde{\mathbf{b}} \cdot \nabla$

Langmuir Probe Data for DIII-D #119919 (J. Boedo)

Electron density and radial particle flux vs. radius -- relative density fluctuations exceed ~20%



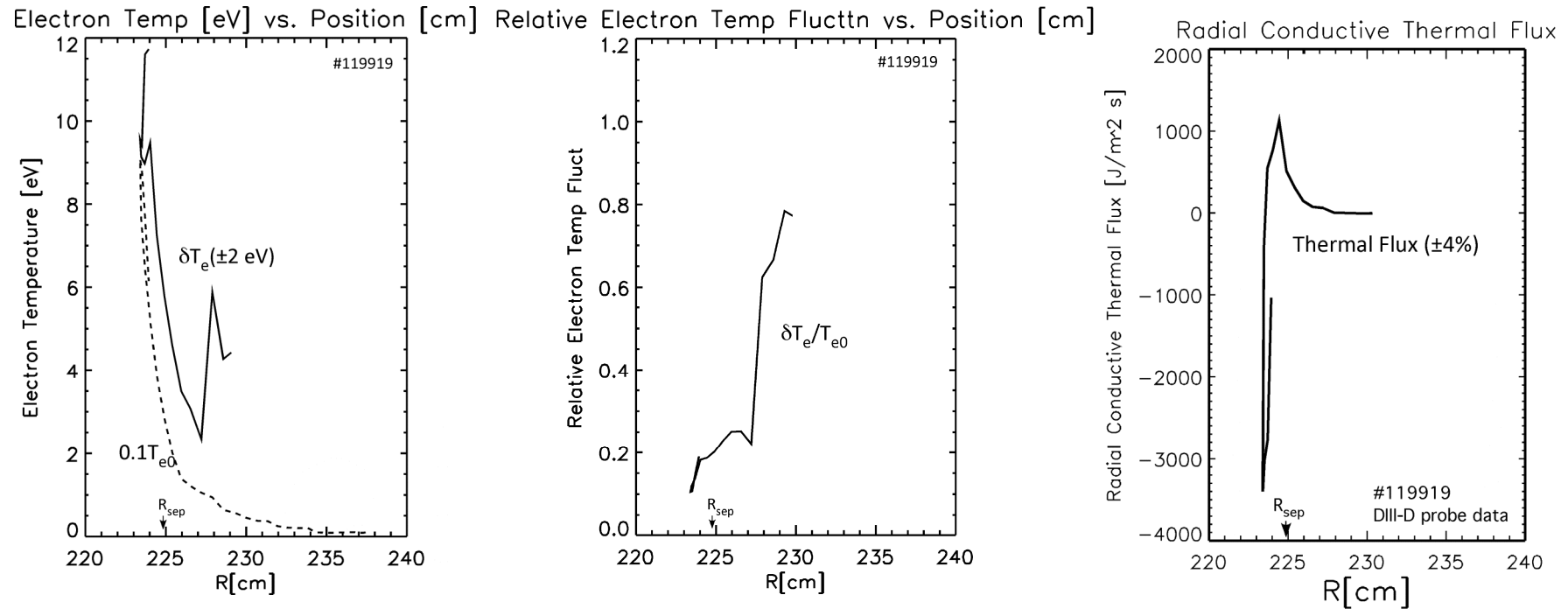
Probe signals decrease
below noise levels for
 $R > 229$ cm.



Typical experimental rms density fluctuations at the separatrix are 24-50%
There is evidence that δn and the radial flux in the midplane peak near R_{sep} as in BOUT results.

Langmuir Probe Data for DIII-D #119919 (J. Boedo)

Electron temperature fluctuations in midplane exceed 10%



Probe signals decrease below noise levels for $R > 229 \text{ cm}$.

Typical experimental rms δT_e fluctuations at the separatrix are 10-25% δT_e and the probe fluxes in the midplane usually peak near the separatrix as in BOUT results.

Summary: As the physics model becomes more complete, the agreement of BOUT results with DIII-D probe data improves

- BOUT algorithmic issues -- control of an odd-even numerical contamination allows us to perform DIII-D simulations
- Comparison of suite of BOUT simulations to shot #119919: peak values in midplane at saturation near R_{sep}

Bout simulation	$\langle \delta N_i \rangle_{rms}$ (10^{18} m^{-3})	$\langle \delta T_e \rangle_{rms}$ (eV)	Radial Particle Flux ($10^{20} / \text{m}^2 \text{ s}$)	D_r (m^2/s) local	Radial Heat Flux $= \frac{3}{2} N_0 \langle \delta \tilde{v}_r \delta \tilde{T}_e \rangle$ ($10^3 \text{ J/m}^2 \text{ s}$)	χ_e (m^2/s), local (conductive)
#1: $\delta T_e = 0$	0.95	N/A	1.8	0.4	N/A	N/A
#2: $\delta T_e \neq 0$ $\kappa_{ e} = 0$	1.0	43	4.3	0.77	54	7.2
#3: $\delta T_e \neq 0$ $\kappa_{ e} \neq 0$	0.58	5.8	1.0	0.17	0.72	0.2
#4: $\delta T_e \neq 0$ $\kappa_{ e} \neq 0$ & $\tilde{\mathbf{b}} \cdot \nabla$	0.9	11	2.8	0.38	3.6	0.8
DIII-D #119919 probe data	2.0	10	11.0	$\sim 0.15\text{-}0.2 \pm$	1.2	$\sim 0.4 \pm$

‡Typical, flux-surface-averaged values for L-mode discharges in DIII-D inferred from UEDGE

B. Cohen, et al., APS DPP 2011